EVALUATION OF COMPUTER MODELS FOR PREDICTING THE FATE AND TRANSPORT OF SALT IN SOIL AND GROUNDWATER

PHASE II REPORT

EVALUATION OF COMPUTER MODELS FOR PREDICTING THE FATE AND TRANSPORT OF SALT IN SOIL AND GROUNDWATER

Phase II Report

Prepared by

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Executive Summary

This report was prepared by MDH Engineered Solutions Corp. (MDH) to document Phase II of a project for Alberta Environment (AE) to evaluate computer codes for predicting the fate and transport of salt (sodium chloride) to facilitate risk-based corrective action.

Phase I of the project recommended five modelling codes for detailed analysis in Phase II. The five codes were chosen from a list of almost 250 codes that were ranked on their strengths, weaknesses, and applicability to the AE salt release scenarios. The five codes recommended for detailed analysis in Phase II were:

1) VS2DTI (USGS);
2) UNSATCHEM (USSL);
3) HYDRUS-2D (USSL-IGWMC);
4) SEVIEW (ESCI); and,
5) CHEMFLOW2000 (OSU).

The principal objective of Phase II was to document the strengths and weaknesses of each code for the specific task of simulating the transport of salt (sodium chloride) at relatively low concentrations, in soil and groundwater in climatic regimes characteristic of the Alberta foothills and prairies. Relatively low concentrations, in this context, is interpreted as concentrations below which density-dependent behaviour can be ignored. This report describes the performance of the five codes for a variety of generic scenarios with varying degrees of complexity. The generic scenarios were derived from a review of typical case histories and are used to illustrate and compare the performance of each of the five selected computer codes. The effects of density-dependent flow and flow through discretely fractured media were not evaluated.

The results of the detailed analysis indicated four of the codes (CHEMFLO, HYDRUS, UNSATCHEM, and VS2DTI) can be readily applied to 1D Tier 2 analysis for the fate/transport of salt. All four codes produced comparable consistent results for the Tier 2 generic scenarios.

SEVIEW (AT 123D, BIOSCREEN and SESOIL) was the only code tested that was designed to predict groundwater recharge from seasonal climatic data. SESOIL is not recommended because of the difficulties encountered in obtaining reasonable estimates of groundwater recharge through tills for the arid western Prairie environment. Nevertheless, AT123D can be used to carry out 1D Tier 2 analysis but without SESOIL has no advantages over the other codes and is limited to homogeneous (or equivalent homogeneous) materials.

For the more complex Tier 3 analysis only VS2DTI and HYDRUS-2D were capable of handling 2D planar and axisymmetric problems. Both codes performed consistently on the 2D generic scenarios but VS2DTI proved more flexible in use.

For cation exchange problems only UNSATCHEM and VS2DTI provided a means of calculation. The two codes use different definitions for selectivity coefficients and are difficult to compare head-to-head. UNSATCHEM is the most sophisticated reactive transport model and readily predicts soil quality parameters such as sodium absorption ratio (SAR) and electrical conductivity (EC).

The detailed comparison resulted in the following recommendations:

1) The revised version of CHEMFLO to be released after March 2003 is recommended as first choice for Tier 2 analysis.

2) UNSATCHEM is recommended for use in Tier 3 assessment where simulation of cation exchange processes and estimates of SAR are requirements.

3) VS2DTI is recommended for application to both 1D column (Tier 2) and 2D planar and axisymmetric (Tier 3) scenarios.

4) SEVIEW is not recommended as a suitable code for screening of salt contaminated sites in Alberta.

5) HYDRUS-2D is judged to be less effective than VS2DI as a tool for Tier 3 analysis.

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1.0 INTRODUCTION

This report was prepared by MDH Engineered Solutions Corp. (MDH) to document Phase II of a project for Alberta Environment (AE) to evaluate computer codes for predicting the fate and transport of salt (sodium chloride) to facilitate risk-based corrective action.

During Phase I of the project (MDH, 2002), a two-level ranking procedure was used to compare almost 250 (247) codes. The first stage of the process was based on review of readily available documentation, some discussion with model developers, and in-house expertise and experience of MDH personnel. This pre-screening stage eliminated over 200 (204) codes, leaving 43 for detailed analysis. The remaining codes were ranked based on 17 objective criteria. The top five codes from the ranking matrix were reviewed in detail for their strengths, weaknesses, and applicability to the AE salt release scenarios. The five codes recommended for detailed analysis in Phase II were:

1) VS2DTI (USGS);

2) UNSATCHEM (USSL);

3) HYDRUS-2D (USSL-IGWMC),

4) SEVIEW (ESCI); and,

5) CHEMFLOW2000 (OSU).

Phase II evaluates the five numerical model codes identified in Phase I for their ability to predict the shallow movement of relatively low concentrations of salt in groundwater. Relatively low concentrations, in this context, is interpreted as concentrations below which density-dependent behaviour can be ignored. This report describes the performance of the five codes for a variety of generic scenarios with varying degrees of complexity. The generic scenarios were derived from a review of typical case histories and are used to illustrate and compare the performance of each of the five selected computer codes. The effects of density-dependent flow and flow through discretely fractured media were not evaluated.

The principal objective of Phase II of the project is to document the strengths and weaknesses of each code for the specific task of simulating the transport of salt (sodium chloride) in soil and groundwater in climatic regimes characteristic of the Alberta foothills and prairies.

2.0 SCOPE OF PHASE II

The scope of the Phase II project was to:

1) Evaluate five numerical computer codes that were highly ranked in the pre-screening process provided in Phase I (MDH, 2002).

2) Develop generic risked-based scenarios derived from typical case histories to illustrate movement of salt from:

   a. Leaks in shallow buried pipelines;

   b. Localized surface sources from periodic use of flare pits; and,

   c. Long term surface sources from highway salt storage piles.

3) Provide a report documenting:

   a. The information requirements to model each scenario;

   b. The ability of each code to simulate the scenarios;

   c. The ease of use of each code; and

   d. The major strengths and weaknesses of each code.

The scope of Phase II did not examine models that could account for density dependent flow or flow through fractured media. In order to have any density effect, there must be a density contrast between the contaminated water and the fresh water. That means that the relative density of the contaminated water must be significantly greater or less than the density of the fresh water. If there is no significant contrast between the contaminated water and the fresh water, then the problem is essentially a normal transport problem involving advection and hydrodynamic dispersion. After discussion

with Alberta Environment, it was concluded that the density gradients would be small for the scenarios being considered, and therefore, density dependent flow could be neglected. Consequently, the models included in the report do not have the ability to simulate density dependent flow. The models apply to circumstance where the concentration of salt in the groundwater does not create large density gradients that would significantly influence the long-term movement of a salt plume. If the site being modelled shows signs of large density gradients, more complex density-dependent codes such as FEMWATER, FEFLOW or SUTRA should be used.

The effects of fracture flow were not included in the study. Clay-rich deposits cover large areas of Canada and the northern United States. The upper layers of these deposits are typically weathered and fractured. Weathering and fracturing can increase the otherwise low hydraulic conductivity of the deposits. Grisak and Pickens (1980) suggest transport of dissolved contaminants in a fractured clay (or porous rock) is expected to be controlled by (1) advection through the fractures; (2) diffusion into the clay matrix between fractures; and (3) retardation processes in both the fractures and matrix. There are only a few field experiments that have estimated the hydraulic fracture aperture and fracture porosity for nonlithified clay-rich or silt-rich deposits. Field studies published by Keller *et. al.* (1986) and McKay *et. al.* (1993) suggest that fractured till could have a representative bulk hydraulic conductivity of up to 3 orders of magnitude greater than the mean value for the unfractured matrix determined from laboratory tests. Often the fractures in the till have been incorporated into numerical models assuming the fractures are frequent and pervasive such that the fractured till acts as an "equivalent porous medium" or epm, and can be accounted for by increasing the hydraulic conductivity. The models included in this report cannot be used for sites that contain media where the individual discrete fractures cannot be represented as part of the soil matrix in terms of a bulk hydraulic conductivity.

3.0 CODE EVALUATION FOR RBCA

The primary basis of the evaluation of the five codes is their suitability for screening sites for risk based corrective action (RBCA). The tiered approach of RBCA is designed to eliminate low-risk sites from further consideration with minimum analysis and expense while retaining high-risk sites for progressively more detailed review. For the purposes of this report, the three tiers of assessment are interpreted as follows:

3.1 Tier 1 Assessment

At this very preliminary level, only an estimate of maximum concentrations and total mass at the point of exposure (POE) and identification of receptors are required. A simple look up table might be sufficient to decide whether the maximum concentration and/or total mass, or the site and/or receptors, justify Tier 2 analysis. Numerical modelling is not usually required at this level.

3.2 Tier 2 Assessment

At this level, the affected porous media needs to be delineated together with determination of the site-specific transport processes and pathways from POE to receptor. Simple 1D column models form the basis for the decision whether or not to proceed to Tier 3 analysis.

3.3 Tier 3 Assessment

For a Tier 3 assessment, the affected porous media needs to be delineated further together with more thorough determination of site-specific transport processes and transport pathways from POE to receptor. More complex 2D or 3D numerical models can be applied at this level to investigate the extent of the problem and evaluate remediation alternatives.

3.3.1 Information Requirements

The same general information is required to complete both a Tier 2 and a Tier 3 analysis. However, more detailed site-specific information should be gathered to complete a Tier 3 analysis.

After a site visit by a professional engineer or geoscientist, the following information should be obtained to complete Tier 2 analysis

1) A professional assessment of the geology to a depth of 5 to 10 m below the zone of contamination;
2) A professional assessment of the location of the potentiometric surface(s);
3) A professional assessment the temporal and spatial extent of salt-sources; and,
4) Site-specific material properties based on literature sources and engineering judgement.

    - The minimum material property data obtained by estimation or measurement should include bulk density, saturated hydraulic conductivity, porosity, water content profile, residual water content, parameters used for predicting the soil water characteristic curves (SWCC), and dispersivities and/or dispersion coefficients.

The following information should be obtained to complete Tier 3 analysis:

1) Borehole information indicating geology to a depth of 5 to 10 m below the zone of contamination;
2) Borehole information adequate to construct 2D site cross-sections;
3) Location of the potentiometric surface(s) and groundwater gradient(s);
4) Site topography and aerial photographs to locate all potential receptors near the site;

    - If aerial photographs or topographic maps do not provide appropriate scale coverage or if the age of the photographs is not indicative of current site conditions, field verification would be necessary to ensure receptors are identified.

5) Material properties based on site-specific testing;

   - The minimum material property data should include bulk density, hydraulic conductivity, porosity, water content profile and residual water content.

6) Material properties based on literature sources and engineering judgement;

   - Parameters used for predicting the soil water characteristic curves (SWCC) and dispersivities and diffusion coefficients could be measured, but are generally taken from literature.

7) Site history sufficient to determine the temporal and spatial extent of salt-sources; and,

8) Soil-salinity data indicating contaminant source concentration and/or contaminant concentration with depth, including EM surveys and groundwater chemical analyses.

Gravels and sands represent high hydraulic conductivity units (aquifers) and tills, clays, and silts comprise the low hydraulic conductivity units (aquitards). Table 3.1 shows typical ranges of hydraulic conductivities for the hydrostratigraphic units researched from literature. MDH provides these values only as a rough guide and strongly advise that modellers should use their own judgement in the application of these values to the specific site being modelled.

Table 3.2 illustrates values of porosity, soil compressibility and specific storage researched from literature. Specific storage is the volume of water released from a unit volume of confined porous medium per unit decline in hydraulic head per unit thickness. Porosity and compressibility of both water and porous medium are related to specific storage as follows (Freeze and Cherry, 1979):

$$S_s = (\alpha + n\beta)\,\gamma_w$$

where: S_s = specific storage [L^{-1}]
α = compressibility of the soil matrix [$F^{-1}L^2$]
β = compressibility of water [$F^{-1}L^2$]
n = porosity [ ]
γ_w = specific weight of water [FL^{-3}]

Table 3.1 - Hydraulic conductivities for typical hydrostratigraphic units.

Hydrostratigraphic Units		Hydraulic Conductivity	
		Upper Limit (m/s)	Lower Limit (m/s)
Surficial stratified deposits	sand		$>1x10^{-7}$ (1)
	Sand	$5x10^{-4}$	$2x10^{-7}$ (4) (7)
	Clay	$2x10^{-9}$	$1x10^{-11}$ (1) (4)
Normally-consolidated till	Oxidized	$4x10^{-6}$	$1x10^{-8}$ (1) (7) (8)
Overconsolidated till	Oxidized	$4x10^{-6}$	$1x10^{-8}$ (1) (7) (8)
	Unoxidized	$2x10^{-6}$	$5x10^{-10}$ (1) (2) (7) (8)
Intertill glaciuofluvial aquifers		$1x10^{-4}$	$3.5x10^{-5}$ (6)
		$6x10^{-3}$	$2x10^{-7}$ (4)
Heavily overconsolidated clay till		$1x10^{-10}$	$1x10^{-11}$ (1) (3)
Buried valley aquifers		$6x10^{-3}$	$2x10^{-7}$ (4)
		$1x10^{-4}$	$1x10^{-5}$ (5)
Bedrock sandstones		$1x10^{-6}$	$1x10^{-9}$ (9)
Bedrock shales		$1x10^{-10}$	$1x10^{-12}$ (9)

Note: The references apply to both the upper and lower limits.
1 Maathuis and van der Kamp (1994a)
2 Site specific data
3 Keller *et al.* (1988) and Keller et al. (1989)
4 Domenico and Schwartz (1998)
5 Maathuis and Schreiner (1982)
6 Maathuis *et al.* (1994)
7 Ho and Barbour (1987)
8 Golder (1997)
9 Freeze and Cherry (1979)

Table 3.2 - Storage properties for typical hydrostratigraphic units.

Hydrostratigraphic Unit		Compressibility (m^2/N)		Porosity (%)		Specific Storage (m^{-1})	
		Upper Range	Lower Range	Upper Range	Lower Range	Upper Range	Lower Range
Surficial stratified deposits	sand	$1.5x10^{-5}$	$1.5x10^{-7}$	50	25	$1.9x10^{-3}$	$6.9x10^{-4}$ (3)
	silt	$1.2x10^{-5}$	$1.2x10^{-7}$	50	35	$1.9x10^{-3}$	$7.4x10^{-4}$ (3)
	clay	$1.5x10^{-6}$	$1.5x10^{-8}$	50	40	$2.7x10^{-3}$	$9.5x10^{-4}$ (1),(2)
Normally consolidated till		$6.9x10^{-7}$	$1.3x10^{-9}$	40	20	$1.3x10^{-4}$	$2.8x10^{-6}$ (1)
Overconsolidated till		$6.9x10^{-7}$	$1.3x10^{-9}$	45	20	$1.3x10^{-4}$	$2.8x10^{-6}$ (1)
Intertill aquifer		$1.5x10^{-6}$	$1.5x10^{-7}$	30	25	$3.8x10^{-4}$	$1.7x10^{-4}$ (3)
Heavily overconsolidated till		$1.2x10^{-7}$	$1.2x10^{-9}$	40	30	$2.7x10^{-4}$	$5.9x10^{-7}$ (2)
Buried valley aquifer		$1.5x10^{-6}$	$5.5x10^{-7}$	35	20	$1.0x10^{-4}$	$3.8x10^{-5}$ (1)
Bedrock sandstone		$1.0x10^{-8}$	$1.0x10^{-10}$	20	5	$1.0x10^{-6}$	$1.0x10^{-8}$ (3)
Bedrock shale		$1.0x10^{-8}$	$1.0x10^{-10}$	15	5	$1.0x10^{-6}$	$1.0x10^{-8}$ (3)

Notes: Compressibility of water at 25°C is 4.8×10^{-10} m^2/N
Soil compressibility values estimated from Dominico and Schwartz (1990) and Canmet (1986)
1 Maathuis and van der Kamp (1994b)
2 Therrien and Sudicky (1996)
3 Freeze and Cherry (1979)

For unconsolidated sediments, the compressibility of the soil is much greater than that of water so the specific storage is controlled by the compression of the pore skeleton. For rigid bedrock aquifers, the opposite is true and the specific storage is controlled by the compressibility of the pore fluid. A reduction in head or pore-pressure results in a release of fluid from storage and a reduction in storage volume as the skeleton collapses. An increase in head or pore-pressure corresponds to an expansion of the storage volume as the skeleton is forced to dilate.

Porosities tend to lie in a relatively narrow range from 5 to 50% (Fetter, 1994; Freeze & Cherry, 1979). Porosity values can be estimated based on typical ranges for different lithologies as cited in the literature. Porosity is a key parameter in contaminant migration and fractured material can exhibit what is called "dual porosity". Clay tills can have matrix porosities up to 50% with a superimposed fracture-porosity of less than 5%. Using the matrix porosity rather than the fracture porosity in contaminant transport

calculations leads to an initial underestimate of the rate of movement since transport takes place rapidly through the fracture network and displaces the matrix pore fluids more slowly. However, none of the evaluated codes have the capability to model "dual porosity" materials.

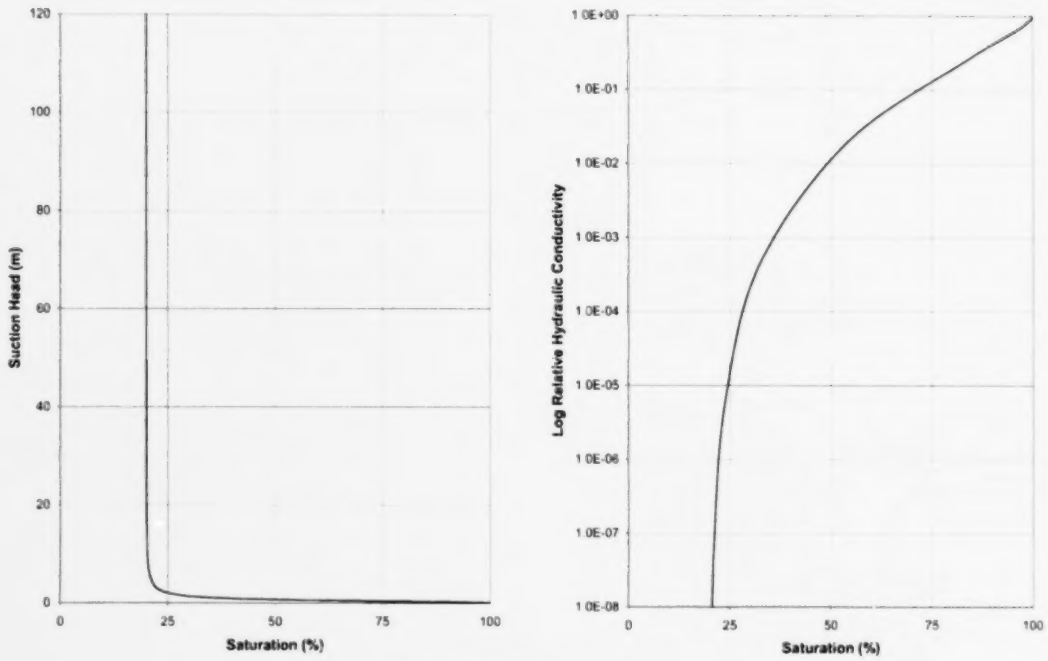
The hydraulic conductivities of soils in the unsaturated zone are lower than the same soil under saturated conditions (below the water table). The reduced moisture contents in the unsaturated zone result in less of the pore-network being available for flow. Suction pressures (negative pressure heads) are preset in the unsaturated zone, with the water table (matric suction = 0) marking the interface between saturated and unsaturated conditions. Hydraulic conductivity is highly dependent on suction pressure when a soil is unsaturated and sands and gravels in the unsaturated state can be barriers to flow. Values for typical coarse and fined grained materials are presented in Table 3.3.

Table 3.3 - Van Genuchten Parameters for prediction of SWCC.

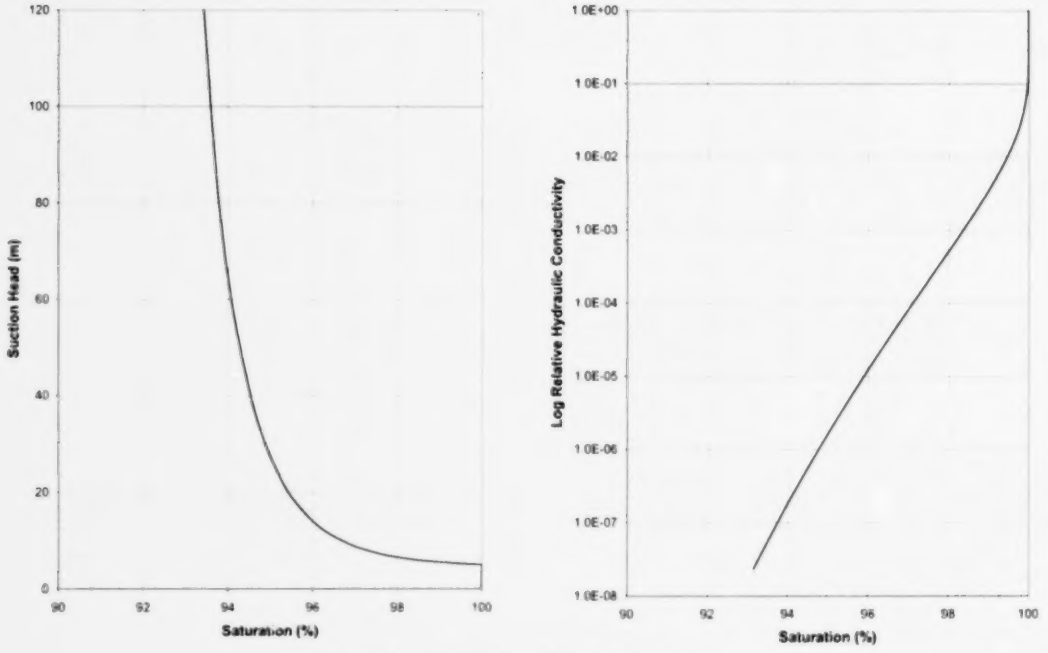
Material	Alpha (m^{-1})	Beta
Fine Grained (clay till)	1.5	1.1
Medium Grained (silt, silty clay)	5	1.8
Coarse Grained (sand)	12	2.7

1 Freeze and Cherry (1979)
2 Domenico and Schwartz (1998)

Typical pressure head versus relative hydraulic conductivity ($K(\theta)/K_{sat}$), degree of saturation (S_e), and moisture content (θ) curves for coarse and fine grained materials are provided in Figure 3.1 (a) and (b), respectively.



(a) Coarse grained material



(b) Fine grained material

Figure 3.1 - Sample soil water characteristic curves.

Sand is easily drained showing a rapid change in saturation for a small suction head increment and a corresponding rapid drop in the relative hydraulic conductivity. The fine-grained material remains almost fully saturated even at large suction heads and only a modest change in relative hydraulic conductivity is associated with drainage. The curves were developed using Van Genuchten parameters based on fitting the results of laboratory tests on similar materials. The program SoilVision (SoilVision Systems Ltd., 1997) and its associated database were used to assist in this process.

Van Genuchten (1980) developed an empirical formula relating hydraulic conductivity and moisture content with negative pressure head:

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{[1 + |\alpha\psi|^{\beta}]^{m}}$$

where: θ = volumetric moisture content
θ_r = residual moisture content
θ_s = saturated moisture content
α = van Genuchten curve-fitting parameter [L^{-1}]
ψ = matric potential or suction pressure [L]
β = van Genuchten curve-fitting parameter
$m = 1 - 1/\beta$

Van Genuchten's function was developed from Mualem's (1978) relationship, used to predict the hydraulic conductivity from moisture retention data:

$$K(S_e) = K_{sat} S_e^{L} [f(S_e) / f(1)]^2 \quad \text{where} \quad f(S_e) = \int_0^{Se} 1 / \psi(x)\, dx$$

where: $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is the degree of saturation
L = is a pore-conductivity parameter or tortuosisy factor

Using Mualem's (1978) model Van Genuchten (1980) derived a closed-form analytical solution to predict the relative hydraulic conductivity (K_r) at a given volumetric water-content:

$$K_r = S_e^{L} \{1 - [1 - S_e^{1/m}]^{m}\}^2$$

Where: S_e can also be written as $[1 + |\alpha\psi|^{\beta}]^{m}$

The confined storage characteristics of the hydrostratigraphic units can be determined by multiplying specific storage by the thickness. On the water capacity against depth curves the specific storage corresponds to the gradient at the water table.

4.0 GENERIC SCENARIOS

The first set of generic scenarios comprised simple 1D columns with a (non-reactive or conservative) tracer contaminant. Analysis of the 1D columns was completed to verify that CHEMFLO, HYDRUS, SEVIEW, UNSATCHEM, and VS2DTI performed consistently using the same input data. The initial comparison was completed using generic data for both homogeneous (uniform) and heterogeneous (layered) systems including both fine and coarse-textured soils.

Additional 2D radial (axisymmetric) analysis was then completed using HYDRUS and VS2DTI on generic scenarios involving more complex sources and boundary conditions.

Finally scenarios involving cation-exchange reactions using UNSATCHEM and VS2DTI were completed to evaluate the ability of these codes to simulate simple reactive transport scenarios involving cation exchange.

4.1 1D Column Scenarios

This phase of modelling was carried out to test the ability of the codes to produce the same results using equivalent or near-identical input. Initially generic simulations were carried out on simple 1D columns with a homogeneous isotropic coarse or fine-grained soil to verify that all five codes produce consistent results. For these analyses it was anticipated that the results would be the same because the geology and mesh-discretization are straightforward and the boundary conditions are simple and unambiguous.

The next step involved increasing the complexity of the 1D columns to include three layers of varying lithology with both saturated and unsaturated flow zones. Such scenarios represent typical Tier 2 screening tasks where the local stratigraphy can be

deduced and generic material-properties can be assigned by an experienced practitioner. From this phase of the analysis, an initial comparison of the codes was made in terms of ease-of-use, flexibility, convergence characteristics, and mass balance performance.

All columns were 30 m high (deep) with a nominal cross section of 1 m^2. The nominal dimensions of the columns, material properties, solute concentrations and application times were kept constant for each simulation. The surface-flux boundary condition was changed depending on whether a coarse or fine-grained soil appeared at the surface to simulate different rates of recharge. In every case the water table was assumed to be at a constant depth, arbitrarily chosen to be 3 m below ground surface (bgs).

All heterogeneous columns were initially run as "flow only" problems to obtain an approximate steady-state initial hydraulic condition for the transport simulation. After a steady-state solution was obtained, a source with a concentration corresponding to brine with a density similar to seawater (30 kg/m^3, 30 g/L or 30,000 mg/L) was applied to the surface of the column for 20 years. After 20 years, the source was removed and the model was run for an additional 20 years to simulate movement of the distributed source.

The source was applied as a constant concentration and constant flux boundary. This boundary condition was chosen because the salt was assumed to enter the column at a rate determined by the ability of infiltration to enter the soil. Neither constant concentration nor constant head boundaries were used because these boundaries generally apply to a ponded source where the inflow rate is determined by the saturated hydraulic conductivity of the soil. This was not likely to be the case for a shallow pipe break, intermittent flare pit or "dry" salt pile. Although the water may be ponded in a flare pit, it was assumed that the ponding would not occur for long enough to maintain the water table at the surface for an extended period.

For 1D columns, it is necessary to specify a second boundary condition at the base of the column. Such boundaries may be specified as free draining or as an advective flow with a user-specified concentration. A third choice is a constant head condition where the flow and mass flux are computed by the code. For the comparative simulations, a

constant pressure head boundary was applied to the base of the 1D columns corresponding to the height of the water table.

The material properties for the generic coarse and fine-grained soils are shown in Table 4.1 and Table 4.2, respectively.

Table 4.1 - Material properties for a homogeneous isotropic coarse-grained soil (sand).

Input Parameter	Value	Units	Dimension
Hydraulic Conductivity	6.9	m/d	L/T
Saturated Water Content (Porosity)	0.25	fraction	dimensionless
Residual Water Content	0.05	fraction	dimensionless
Van Genuchten parameter alpha	12	1/m	1/L
Van Genuchten parameter beta	2.7	exponent	dimensionless

The material properties in Table 4.1 were chosen to be characteristic of a clean medium-grained sand. Such sand horizons commonly occur in glaciofluvial channels.

Table 4.2 - Material properties for a homogeneous isotropic fine-grained soil (clay till).

Input Parameter	Value	Units	Dimension
Hydraulic Conductivity	8.6×10^{-4}	m/d	L/T
Saturated Water Content (Porosity)	0.36	fraction	dimensionless
Residual Water Content	0.30	fraction	dimensionless
Van Genuchten parameter alpha	1.5	1/m	1/L
Van Genuchten parameter beta	1.1	exponent	dimensionless

The materials in Table 4.2 were chosen to be characteristic of a poorly-sorted homogeneous till with a silty-clay matrix. It is assumed that the till is a single-porosity porous medium. A dual porosity medium with a component of fracture flow is not considered. For such a material, a considerably lower porosity might be used to characterize the solute interaction with the fracture-porosity component alone.

The solute transport parameters used in the generic models are listed in Table 4.3. Diffusion coefficients for porous media were estimated by multiplying the self-diffusion coefficient by porosity. A single (low) value was applied for longitudinal dispersivity. Dispersivity is generally regarded as a scale-dependent property and the value used is appropriate on the tens-of-metres scale. For solute transport on a scale of hundreds of metres, a second value is included in the table.

Table 4.3 - Solute transport parameters.

Input Parameter	Value	Units	Dimension
Diffusion Coefficient (Cl^-)	4.4×10^{-5}	m^2/d	L^2/T
Diffusion Coefficient (Na^+)	2.9×10^{-5}	m^2/d	L^2/T
Diffusion Coefficient (Ca^{2+})	1.7×10^{-5}	m^2/d	L^2/T
Longitudinal Dispersivity (10 m scale)	0.4	m	L
Longitudinal Dispersivity (100 m scale)	4.0	m	L

Dispersivity is the property of a porous medium that characterizes mechanical mixing in a flow field. Longitudinal dispersivity (α_L) quantifies mixing in the direction of flow and transverse dispersivity (α_T) characterizes mixing normal to the mean flow direction. In common with hydraulic conductivity, dispersivity varies with the scale of measurement. A reasonable rule of thumb is that macroscopic dispersion (field scale) is approximately 2 orders of magnitude greater than microscopic dispersion (lab scale). At the lab column scale, longitudinal dispersivity is typically between 0.01 and 1.0 cm. In field studies, values from 0.1 to 2.0 m are observed over short distances in well-controlled experiments. Longitudinal dispersivity values >10 m are reported over longer distances, but data is very sparse and based on the back-analysis of documented plumes.

The famous Borden experiment (Sudickey, 1986; Mackay *et al.*, 1986) conducted field scale dispersivity measurements. The study found that medium-grained, fine-grained, and silty fine-grained sand, gave a field dispersivity value of 0.45 m over a travel distance 58 m. Transverse dispersivity is generally at least an order of magnitude smaller than longitudinal dispersivity. Table 4.4 summarizes the information used to estimate dispersivities.

Table 4.4 - Solute transport parameters.

Dispersivity Scale	Value Range (m)
Laboratory homogeneous sand column experiments	10^{-4} to 10^{-2}
Naural-gradient tracer field experiments	10^{-2} to 10^{-0}
Empirical fitting or matching of field plumes	10^{0} to 10^{2}

It is well established that the apparent dispersivity, used to compute the dispersion coefficient in the advection-dispersion equation, exhibits scale effects. The apparent dispersivity grows with the plume size until the size of the plume reaches 10-15 times the size of the largest scale of heterogeneity (Howington *et al.*, 1997). For typical sand aquifers, interpreting the largest heterogeneity as lenticular bodies with a length scale of 1-5 m, an appropriate choice for dispersivity would seem to be about 10 to 50 m.

The information common to all the codes is provided in Tables 4.1 to 4.3. However, each code requires the input data in a slightly different form. Therefore, a detailed description of the information specific to each modelling code is provided in Appendix A.

4.1.1 Homogeneous Isotropic Coarse-Grained Soil Column – Surface Source

The boundary conditions utilized in the modelling of the uniform isotropic coarse-grained soil column are provided in Table 4.5. An exit-solution concentration of zero was applied to the base of the column. It was assumed that the base of the column was below the zone of contamination, and no contaminant would exit in the outflow during the simulation period.

Table 4.5 - Boundary conditions for a homogeneous isotropic coarse-grained soil column (surface source).

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4×10^{-5}	m/d
Base Boundary for Flow	Constant Head	27	m
Surface Boundary for Solute (0-20 years)	Solute Concentration	30	kg/m^3
Surface Boundary for Solute (20-40 years)	Solute Concentration	0	kg/m^3

The surface flux is characteristic of infiltration rates into sandy surfaces under climatic conditions expected in the western Canadian prairies. Figure 4.1 illustrates the concentration distribution of the contaminant plume after 20 years of source application for CHEMFLO, HYDRUS, UNSATCHEM, and VS2DI.

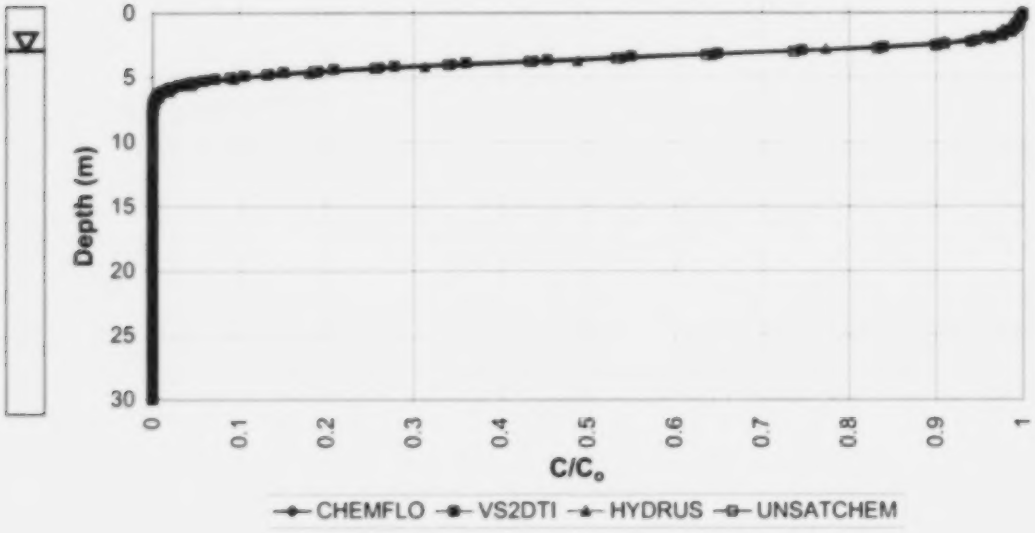


Figure 4.1 - Concentration versus depth profiles after 20 years of source application (homogeneous isotropic coarse-grained soil column).

Figure 4.1 shows that the modelling results for CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI correspond very closely. For the coarse-grained soil column, the plume has penetrated to a depth of approximately 6.8 metres (from 6.7 to 6.8 m) after 20 years of continuous source applied to the surface. The peak concentration is approaching the source concentration of 30 kg/m^3. Plume penetration depth is arbitrarily defined as the depth where concentration exceeds 1 kg/m^3 or C/Co > 0.033. Detailed input and output data for the simulations can be found in Appendix A and Appendix B, respectively.

Results are not shown for SEVIEW (SESOIL combined with AT123). SESOIL computes a water balance from seasonal climatic data and applies the groundwater recharge to the surface of the AT123 flow model. SESOIL is designed as a screening program for low concentration organic contaminants in relatively permeable surface soils. The

application of SESOIL and AT123 are limited to homogeneous materials and can only provide a Tier 1 level of screening. SESOIL was unsuccessful in predicting positive recharge for raw climatic data from the western Canadian prairies. After considerable data manipulation, it was possible to generate positive groundwater recharge but it proved extremely difficult to apply SESOIL to commonly occurring low-permeability soils (e.g. tills). For these reasons, comparative evaluation of SEVIEW and the other codes was not feasible.

4.1.2 Homogeneous Isotropic Fine Grained Soil Column – Surface Source

The boundary conditions utilized in modelling the homogeneous fine-grained soil column are provided in Table 4.6. An exit-solution concentration of zero was applied to the base of the column, because it was assumed that the base of the column was below the zone of contamination and no contaminant would exit in the outflow during the simulation period.

Table 4.6 - Boundary conditions for a homogeneous isotropic fine grained soil column (surface source).

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	1.0×10^{-5}	m/d
Base Boundary for Flow	Constant Head	27	m
Surface Boundary for Solute (0-20 years)	Solute Concentration	30	kg/m^3
Surface Boundary for Solute (20-40 years)	Solute Concentration	0	kg/m^3

The surface flux value is considered characteristic of infiltration rates into till surfaces under climatic conditions expected in the western Canadian prairies. Figure 4.2 illustrates the concentration of the contaminant plume after 20 years of source application.

Figure 4.2 shows that the modelling results for CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI correspond very closely. For the fine-grained soil column, the plume has penetrated to a depth of approximately 2.0 metres (1.8 to 2.1 m) after 20 years of

continuous source applied to the surface. The C/C° is approximately 0.36. Detailed input and output data is provided in Appendix A and Appendix B, respectively.

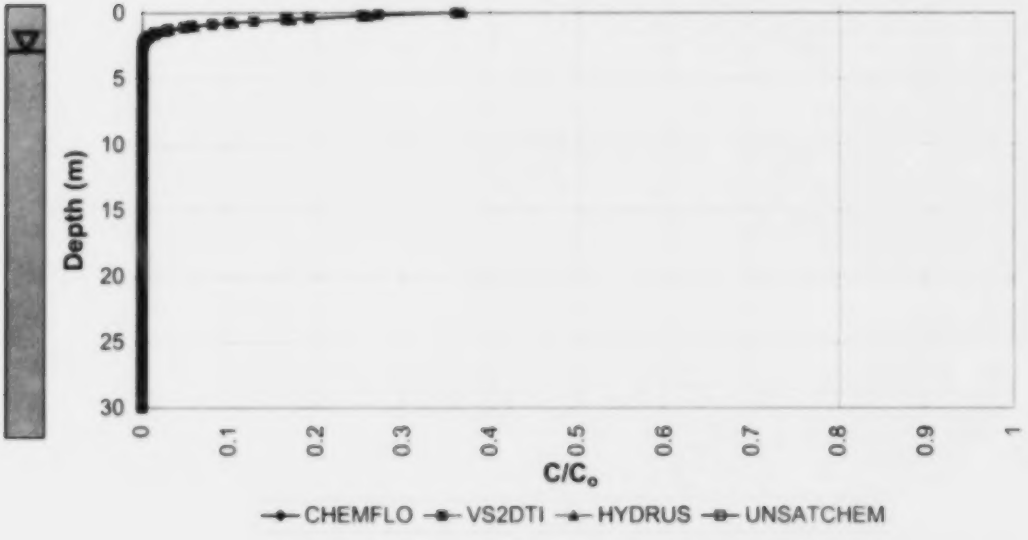


Figure 4.2 - Concentration versus depth profiles after 20 years of source application (homogeneous isotropic fine-grained soil column).

4.1.3 Heterogeneous (Layered Fine-Coarse-Fine) Isotropic Soil Column – Surface Source

The boundary conditions utilized in the modelling of the isotropic, layered fine-coarse-fine soil column are provided in Table 4.7. An exit-solution concentration of zero was applied to the base of the column, because it was assumed that the base of the column was below the zone of contamination, and no contaminant would exit in the outflow during the simulation period.

Table 4.7 - Boundary conditions for an isotropic, layered fine-coarse-fine soil column (surface source).

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	1.0×10^{-5}	m/d
Base Boundary for Flow	Constant Head	27	m
Surface Boundary for Solute (0-20 years)	Solute Concentration	30	kg/m^3
Surface Boundary for Solute (20-40 years)	Solute Concentration	0	kg/m^3

The surface flux utilized in the models is characteristic of infiltration rates into till surfaces under climatic conditions expected in the western Canadian prairies. Figure 4.3 illustrates the concentration of the contaminant plume after 20 years of source application.

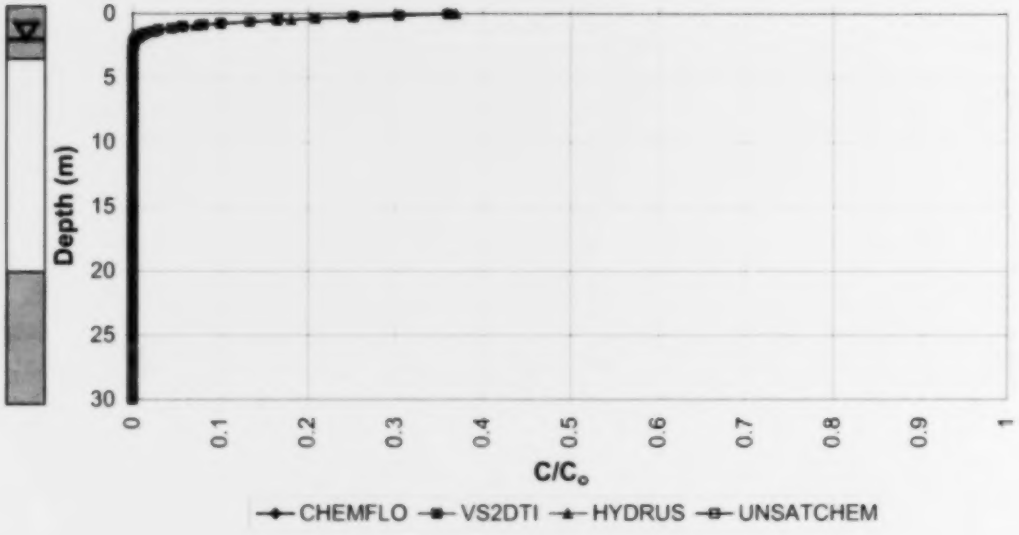


Figure 4.3 - Concentration versus depth profiles after 20 years of source application (layered fine-coarse-fine soil column).

Figure 4.3 shows that the modelling results for CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI correspond very closely. For the fine-coarse-fine soil column, the plume has

penetrated to a depth of approximately 2.0 m (from 1.8 to 2.1 m) after 20 years of continuous source applied to the surface. The C/C° is about 0.36. The result is very similar to the uniform fine-grained soil because the plume has not reached the first fine-coarse interface (at a depth of 4 m) after the 20 years of simulation. Detailed input and output data is provided in Appendix A and Appendix B, respectively.

4.1.4 Heterogeneous (Layered Coarse-Fine-Coarse) Isotropic Soil Column – Surface Source

The boundary conditions utilized in the modelling of the isotropic, layered coarse-fine-coarse soil column with a surface source are provided in Table 4.8. An exit-solution concentration of zero was applied to the base of the column, because it was assumed that the base of the column was below the zone of contamination, and no contaminant would exit in the outflow during the simulation period.

Table 4.8 - Boundary conditions for an isotropic, layered coarse-fine-coarse soil column (surface source).

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4×10^{-5}	m/d
Base Boundary for Flow	Constant Head	27	m
Surface Boundary for Solute (0-20 years)	Solute Concentration	30	kg/m^3
Surface Boundary for Solute (20-40 years)	Solute Concentration	0	kg/m^3

The surface flux applied to the soil column is characteristic of infiltration rates into sandy surfaces under climatic conditions expected in the western Canadian prairies. Figure 4.4 illustrates the concentration of the contaminant plume after 20 years of source application.

Figure 4.4 shows that the modelling results for CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI correspond very closely. For the coarse-fine-coarse soil column, the plume has penetrated to a depth of about 6.2 m (from 6.1 to 6.2 m) after 20 years of continuous source applied to the surface. The peak concentration is close to the source

concentration at about 30 kg/m^3. The plume penetration depth is approximately 0.5 m higher than the uniform coarse soil case because the plume is slowed at the first coarse-fine interface at a depth of 4 m. Detailed input and output data is provided in Appendix A and Appendix B, respectively.

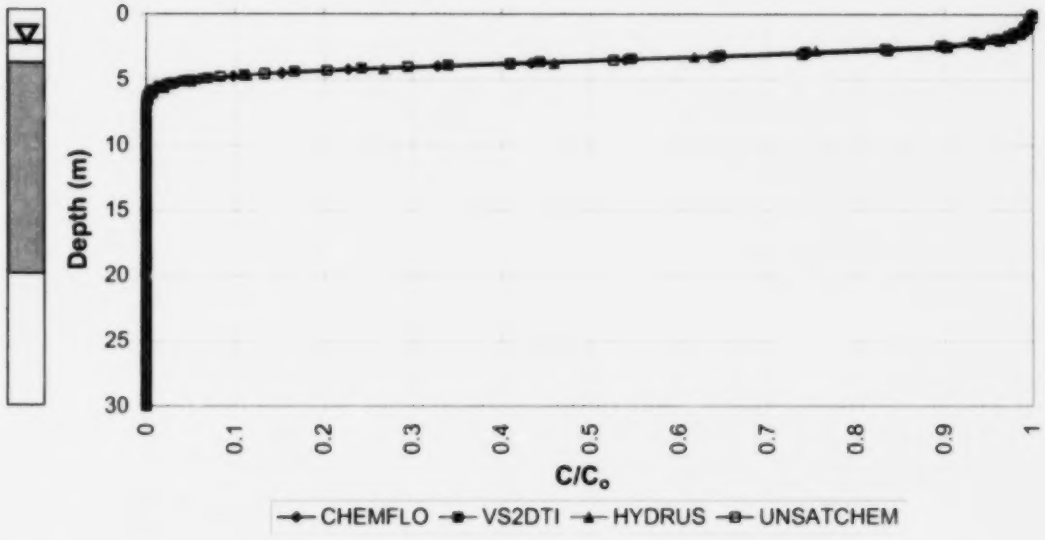


Figure 4.4 - Concentration versus depth profiles after 20 years of source application (layered coarse-fine-coarse soil column).

Figure 4.5 shows the progress of the contaminant plume over a period of 40 years (20 years of source application). Profiles after 5, 10, 15, 20, 25, 30, 35 and 40 years are provided in Figure 4.5. The results are plotted for UNSATCHEM but are very similar for all codes. Over the period of source application, the leading edge of the plume sinks from surface to 6.2 m. After the source is removed, the profiles show the broadening and attenuation of the plume peak over time from an initial value of 30 kg/m^3 (or C/Co = 1.00 at surface) to 13 kg/m^3 (or C/Co = 0.43 at 4.3 m depth after 40 years). The leading edge of the plume has reached a depth of 8.6 m after 40 years of simulation.

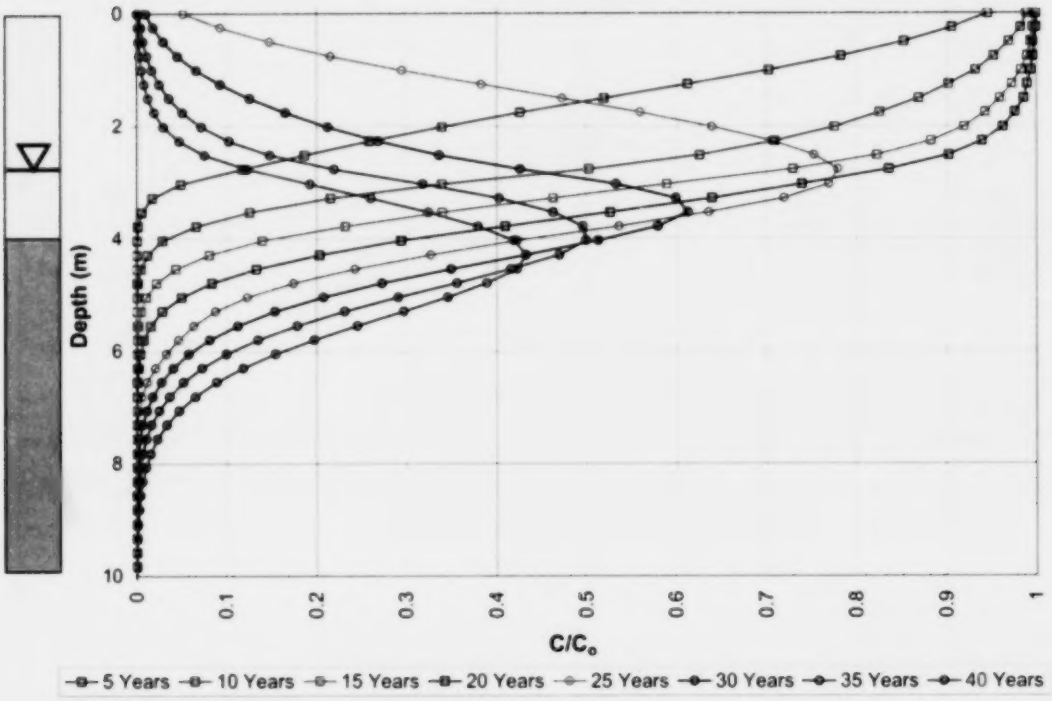


Figure 4.5 - UNSATCHEM concentration versus depth profiles (layered coarse-fine-coarse soil column with 20 year source application).

4.1.5 Isotropic Layered Coarse-Fine-Coarse Soil Column – Distributed Source

The boundary conditions utilized in the modelling of the isotropic, layered coarse-fine-coarse soil column are provided in Table 4.9. An exit-solution concentration of zero was applied to the base of the column because it was assumed that the base of the column was below the zone of contamination, and no contaminant would exit in the outflow during the simulation period. The distributed source varied linearly from 20 kg/m^3 at surface to 30 kg/m^3 at a depth of 3 m. The source then reduced linearly to zero at a depth of 10 m.

Table 4.9 - Boundary conditions for isotropic layered course-fine-course soil column (distributed source).

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4×10^{-5}	m/d
Base Boundary for Flow	Constant Head	27	m
Surface Boundary for Solute (0 years)*	Solute Concentration	20	kg/m^3
3 m Depth Boundary (0 years)*	Solute Concentration	30	kg/m^3
10 m Depth Boundary (0 years)*	Solute Concentration	0	kg/m^3
Surface Boundary for Solute (20-40 years)	Solute Concentration	0	kg/m^3

* Note: Initial concentrations varied linearly between depths.

The surface flux is characteristic of infiltration rates into sandy surfaces under climatic conditions expected in the western Canadian prairies. Figure 4.6 illustrates the concentration of the contaminant plume after 20 years.

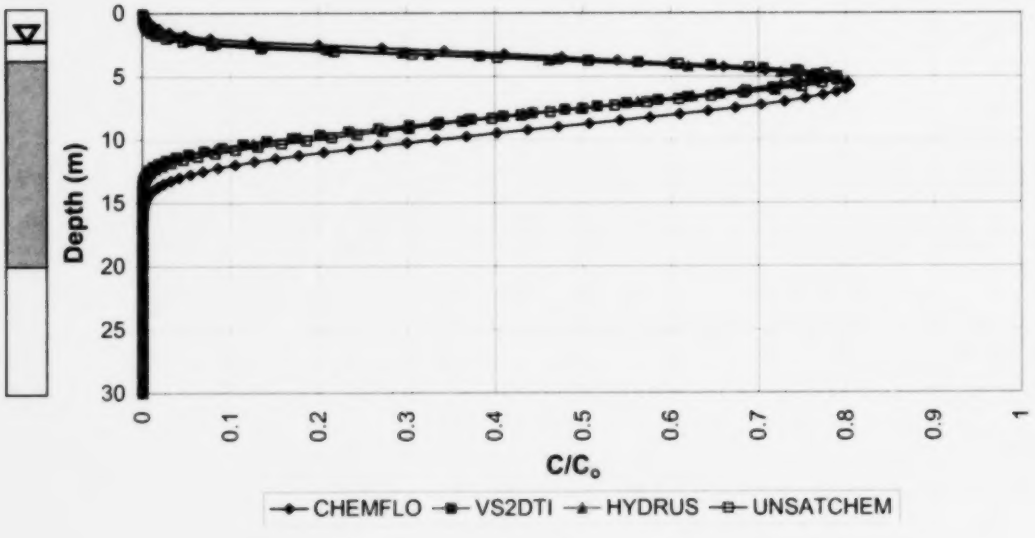


Figure 4.6 - Concentration versus depth profile for distributed source after 20 years (layered coarse-fine-coarse soil column).

After 20 years of simulation, the source distributions predicted by CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI were all similar, with a peak relative concentration (C/Co) of 0.77 (from 0.73 to 0.83) at a depth of 5.2 metres (5.1 to 6.5 m). CHEMFLO appears to predict slightly faster migration, with the peak concentration deeper than predicted using the other codes (Figure 4.6). This is likely due to small differences in the location of the distributed source relative to the model mesh or grid in the different simulations. Detailed input and output data is provided in Appendix A and Appendix B, respectively.

4.2 2D Axisymmetric (Radial) Scenarios

After the initial comparison and verification of consistency was completed on the 1D soil columns, a comparison was made of the ability of the codes to provide a Tier 3 site assessment. The pipeline, flare pit, and salt pile scenarios were simulated using 2D axisymmetric models with three material layers. Of the five codes, only HYDRUS-2D and VS2DTI were capable of this level of analysis. Some variation in results between codes was anticipated for these scenarios because each program has different input parameters and specification details for mesh construction, boundary conditions and material properties.

4.2.1 Pipeline Break Scenario

The pipeline scenario was modeled for an isotropic, heterogeneous (coarse-fine-coarse layered) soil section. The pipe (with a nominal diameter of 500 mm) was placed with the centreline at a depth of 1.25 m below ground surface. The pipeline scenario was modelled assuming the pipe break to be a finite length (500 mm), with a constant leakage rate and duration. Because of the limitations of an axisymmetric model, the pipe break was limited to being modeled as a point source. The source appears as a "cylinder" in the model, with a height and diameter of 500 mm as shown in Figures 4.7 and 4.8.

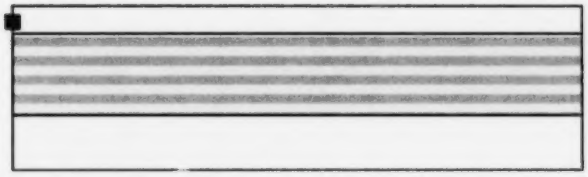


Figure 4.7 - 2D schematic of pipeline break (red block indicates break location).

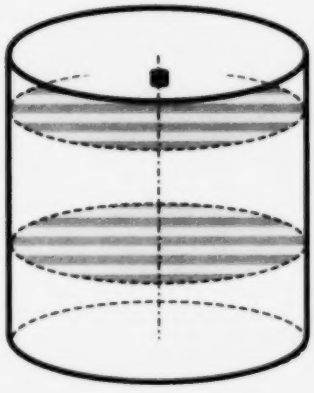


Figure 4.8 - 3D radial schematic of pipeline break (red block indicates break location).

The boundary conditions utilized in modelling the pipeline break in the layered coarse-fine-coarse soil are provided in Table 4.10.

Table 4.10 - Boundary conditions for pipeline break scenario.

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4×10^{-5}	m/d
Radial Boundary for Flow – Upper Aquifer	Constant Total Head	-3	m
Radial Boundary for Flow – Lower Aquifer	Constant Total Head	-4	m
Flow from Pipe into System	Constant Flow	0.02	m^3/d
Pipe Boundary for Solute (0 - 1 years)	Solution Concentration	30	kg/m^3
Pipe Boundary for Solute (1 - 11 years)	Solution Concentration	0	kg/m^3

Figure 4.9 illustrates that after 1 year of leakage, HYDRUS and VS2DTI produce similar predictions for the profile and relative concentration of the plume. The peak concentration beneath the pipeline break occurs at a depth of approximately 2.5 m. Both codes predict salt concentrations of about 5 to10% of the source at the ground surface.

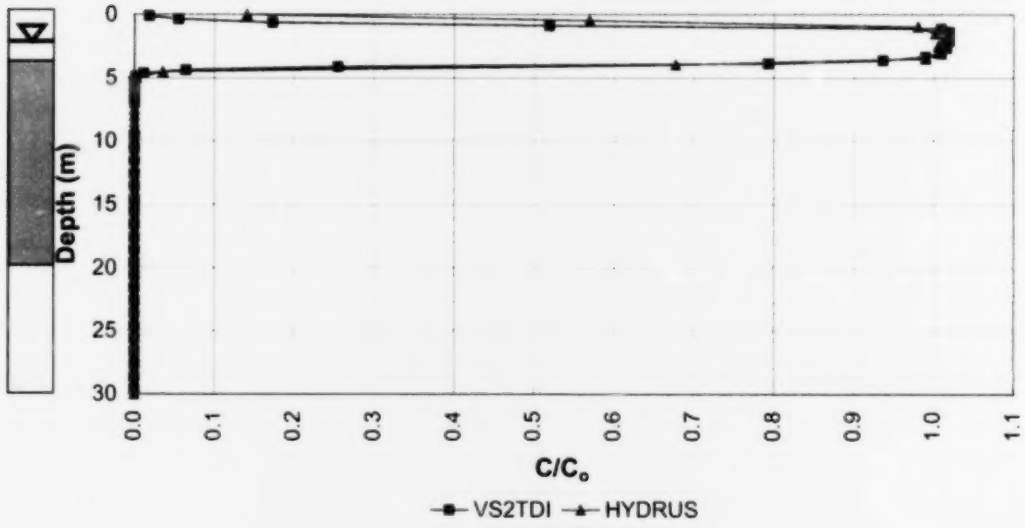


Figure 4.9 - Concentration versus depth for pipeline break after 1 year.

Figure 4.10 (HYDRUS) and Figure 4.11 (VS2DTI) show that the plume extends to a radial distance of approximately 3.0 m after 1 year of leakage. After this time, the source concentration was turned off and the simulation was run for another 10 years. Detailed simulation results are provided in Appendix C.

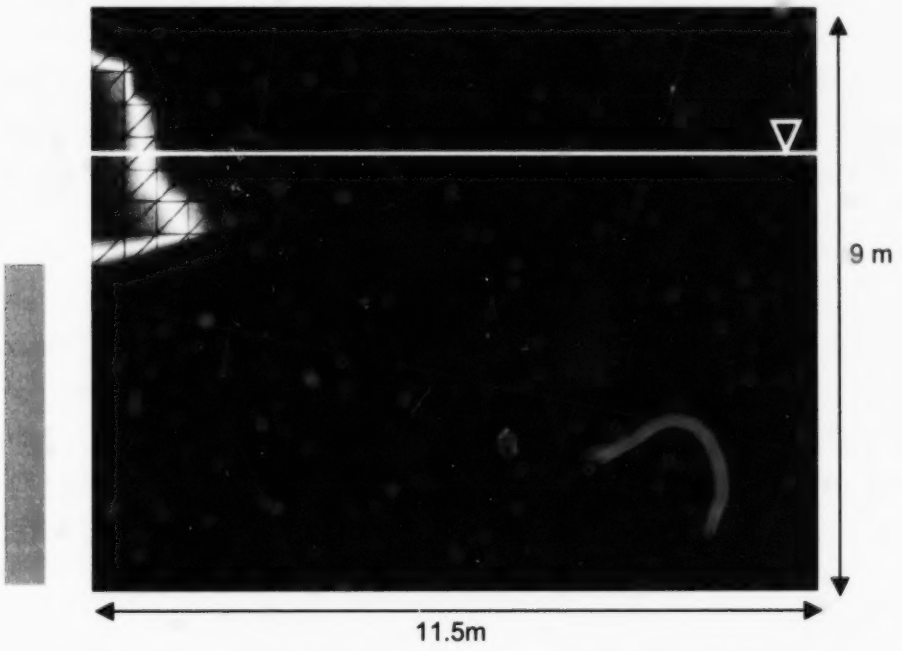


Figure 4.10 - 2D plume from pipeline break after 1 year of leakage (HYDRUS).

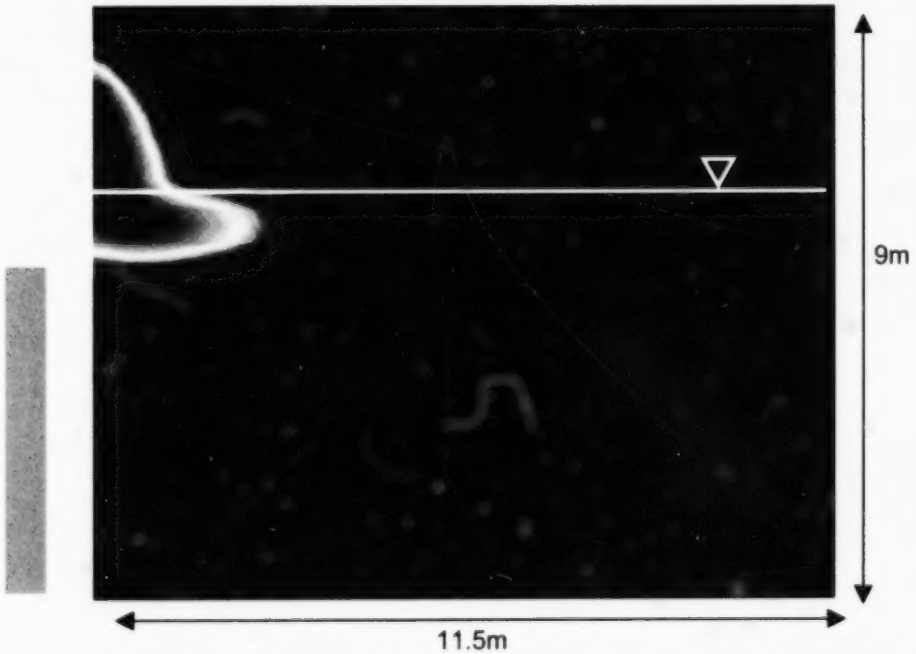


Figure 4.11 - 2D plume from pipeline break after 1 year of leakage (VS2DTI).

4.2.2 Flare Pit Scenario

The flare pit scenario was modelled for a isotropic, heterogeneous (coarse-fine-coarse layered) soil section. The flare pit was assumed to be 10 m in diameter at the base, 12 m in diameter at the surface and 2 m deep. A constant head boundary was placed at the base of the flare pit during periods when salt water was assumed to be released into the pit. This scenario must therefore be modelled with an irregular (non-rectangular) domain geometry. The mesh generator provided with HYDRUS-2D only allows a rectangular mesh. An additional mesh generator is available for purchase, however, it was not purchased during this stage of the study. For this reason, only VS2DTI could be used to complete the flare pit simulation. Schematics of the scenario are shown in Figures 4.11 and 4.12.

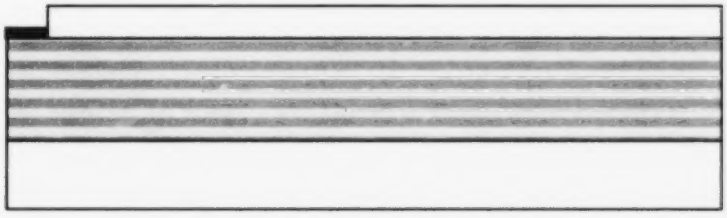


Figure 4.12 - 2D schematic of flare pit (red block indicates pit source).

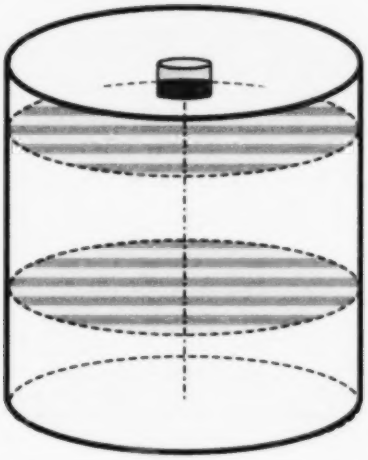


Figure 4.13 - 3D radial schematic of flare pit (red block indicates pit source).

The boundary conditions utilized for modeling the flare pit in an isotropic, layered coarse-fine-coarse soil section are provided in Table 4.11. The concentration of the water discharged into the pit was assumed to be equal to the concentration of seawater. The salt water source concentration of 35 kg/m^3 was applied to the base of the pit for 30 days and then removed for 335 days. This intermittent cycle was repeated for 10 years.

Table 4.11 - Boundary conditions for flare pit scenario.

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4×10^{-5}	m/d
Radial Boundary for Flow – Upper Aquifer	Constant Total Head	-3	m
Radial Boundary for Flow – Lower Aquifer	Constant Total Head	-4	m
Pit Boundary (30 day discharge periods)	Constant Total Head	-1.5	m
Pit Boundary (335 day empty periods)	Constant Flux	5.4×10^{-5}	m/d
Pit Boundary for Solute (30 day discharge periods)	Solution Concentration	35	kg/m^3
Pit Boundary for Solute (335 day empty periods)	Solution Concentration	0	kg/m^3

The results from the VS2DTI model after eight cycles over a period of eight years are provided in Figure 4.14. The modelling results indicates the intermittent recharge to the pit has developed a continuous saturated zone in the upper sand aquifer and the plume has migrated to a radial distance of more than 50 m. The peak concentration in the plume is close to the applied source value of 35 kg/m^3. The salt has migrated more than 2 m vertically into the till beneath the surface aquifer. Adjacent to the pit, high salt concentrations are predicted in the unsaturated zone and at the surface.

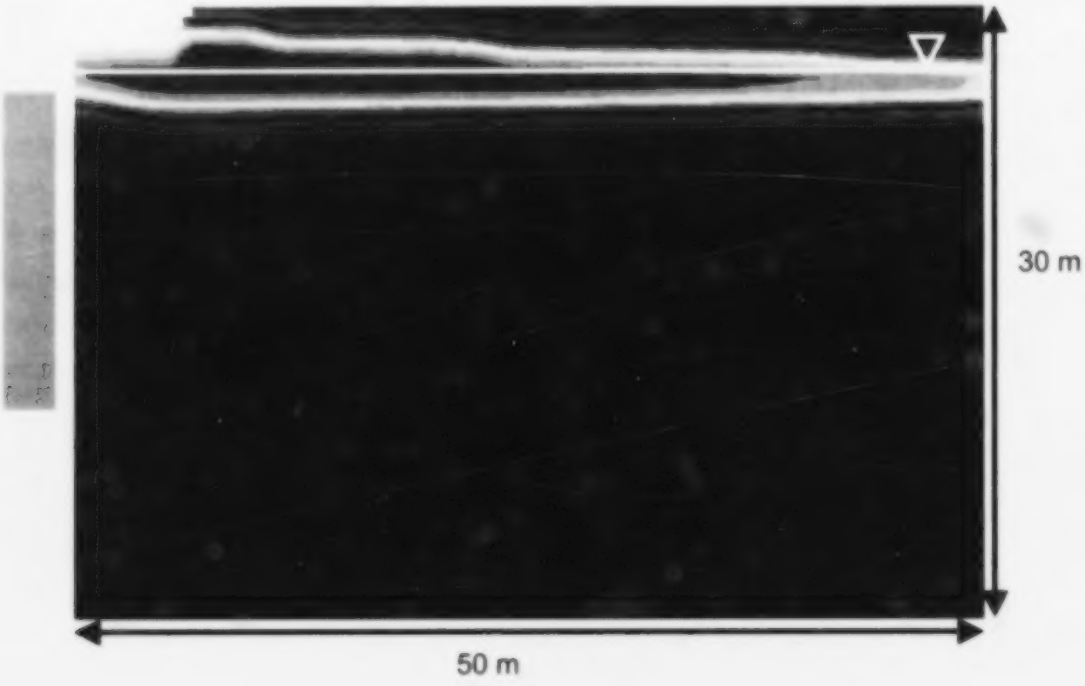


Figure 4.14 - 2D plume from a flare pit after 8 years of operation (VS2DTI)

4.2.3 Salt Pile Scenario

The salt pile was modelled for a isotropic, heterogeneous (coarse-fine-coarse layered) soil section. The salt pile was modelled as a 10 m radius source. Salt was assumed to enter the ground dissolved in surface infiltration. Because of the limitations of an axisymmetric model, the salt pile was limited to being modelled as a circular surface source. The source appears as a disc on the surface of the model, as shown in Figures 4.15 and Figure 4.16.

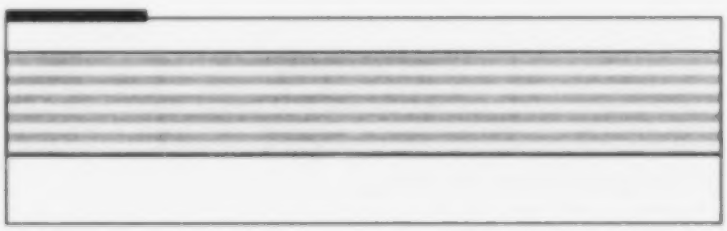


Figure 4.15 - 2D schematic of salt pile (red block indicates pile).

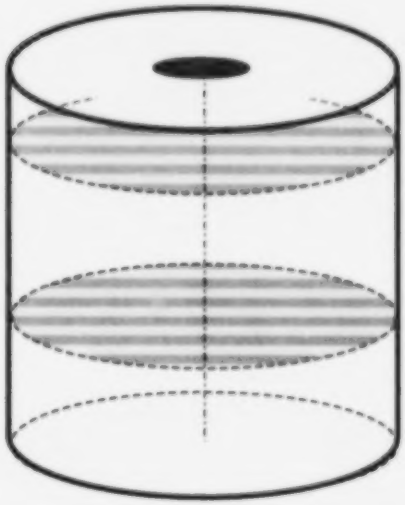


Figure 4.16 - 3D radial schematic of salt pile (red block indicates pile).

The boundary conditions utilized for modelling the isotropic, layered coarse-fine-coarse soil beneath the salt pile are provided in Table 4.12. The concentration of the infiltrating solution was assumed to be close to seawater (30 kg/m^3). It was assumed that leakage from the salt pile continued at the same location for 20 years. After 20 years, the source was removed and the scenario was simulated for an additional 20 years allowing the plume to dissipate.

Table 4.12 - Boundary conditions for salt pile scenario.

Boundary	Boundary Type	Value	Units
Surface Boundary for Flow	Constant Flux	5.4 x 10^{-5}	m/d
Radial Boundary for Flow – Upper Aquifer	Constant Total Head	-3	m
Radial Boundary for Flow – Lower Aquifer	Constant Total Head	-4	m
Pile Boundary for Solute (0 - 20 years)	Solution Concentration	30	kg/m^3
Pile Boundary for Solute (20 - 40 years)	Solution Concentration	0	kg/m^3

The results from the HYDRUS and VS2DTI models are shown in Figure 4.17 and Figure 4.18. The results indicate that the two codes produced essentially the same results for this scenario. Figure 4.17 shows that the salt plume has extended to a depth of approximately 6.0 m, after 20 years.

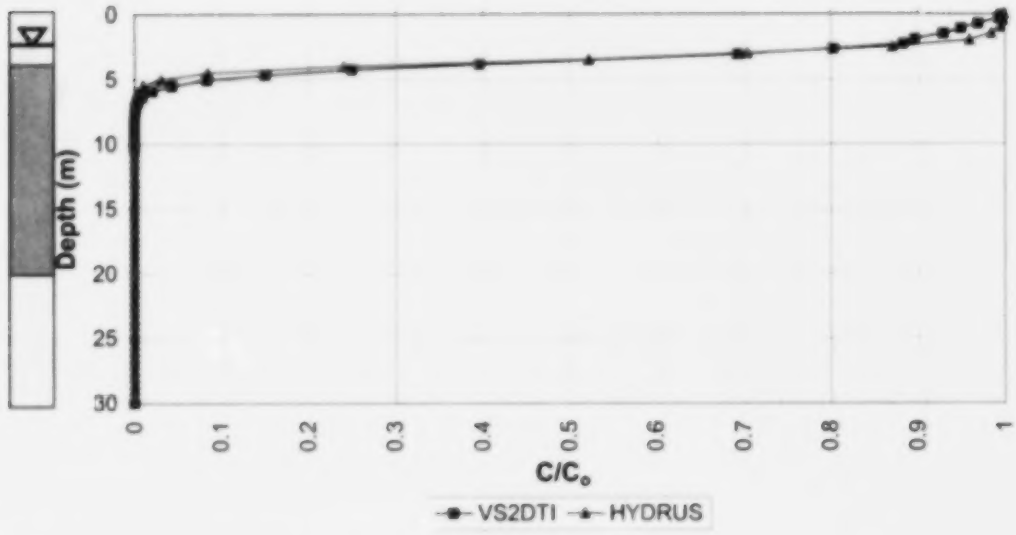


Figure 4.17 - Concentration versus depth for salt pile scenario after 20 years.

Figure 4.18 (HYDRUS) and Figure 4.19 (VS2DTI) show that the plume extends to a radial distance of approximately 5.0 m away from the site after 20 years of source infiltration. The contrast between the salt pile source (driven by infiltration alone) and the "ponded" flare pit source for the same geology, shows that the spatial and temporal distribution of the source is critical information.

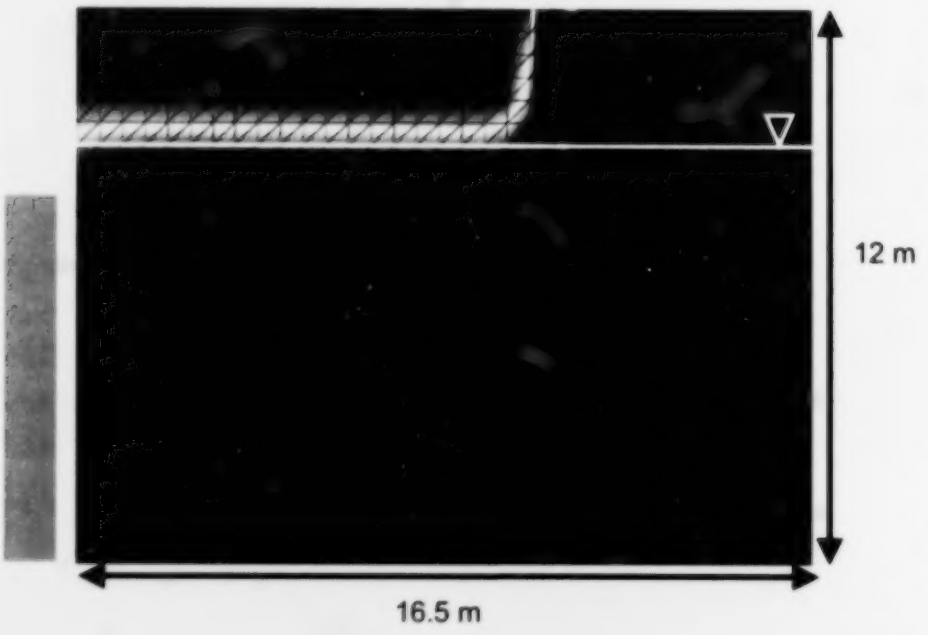


Figure 4.18 - 2D plume for salt pile after 20 years of source application (HYDRUS).

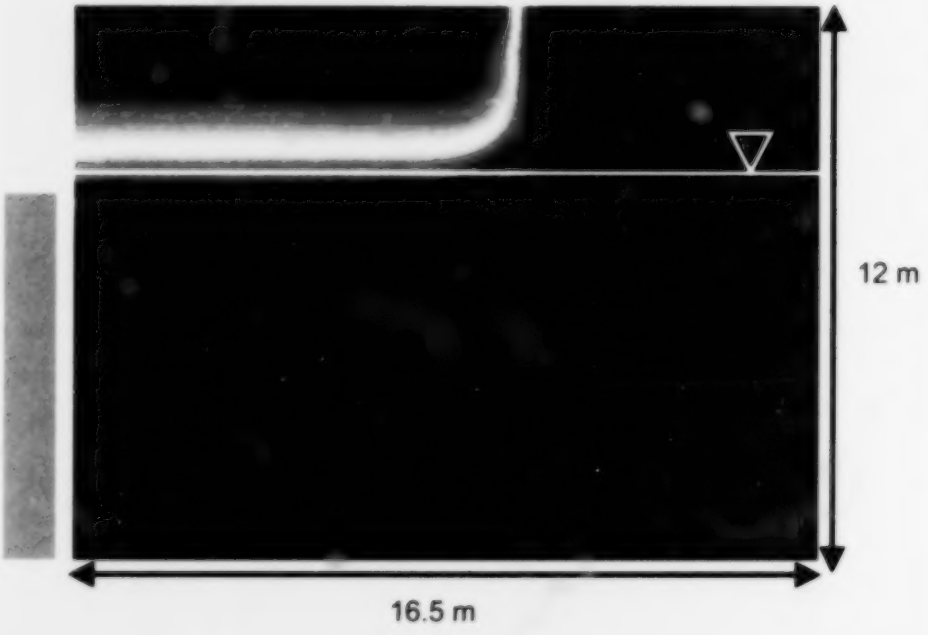


Figure 4.19 - 2D plume for salt pile after 20 years of source application (VS2DTI).

4.3 Reactive Transport Scenarios

In many soils the solid phase carries a net negative surface charge. For clay minerals this charge is a result of isomorphous substitution, where structural cations of higher valence are replaced by cations of lower valence (e.g. Si^{4+} is replaced by Al^{3+}). As a result, clay minerals have a permanent negative surface charge. Oxides and soil organic matter (SOM) also have charged surfaces: With increasing pH, H^+ is dissociated from oxide surfaces or from organic functional groups resulting in a negative charge. Because dissociation increases with pH and ionic strength, such charge is variable charge as opposed to the permanent charge of clays. At low pH values, oxides may bind H^+, which results in a positive surface charge. The pH values at which positively charged groups quantitatively equal negatively charged groups (i.e. the net surface charge is zero) are called zero point of charge (ZPC).

In soils, the overall electroneutrality is maintained by an excess of electrostatically attracted counterions in proximity to the charged surface (Figure 4.20). In the case of negatively charged surfaces, a diffuse double layer will result where cations are in excess of anions. The excess ions, termed exchangeable cations, may be exchanged with neutral salts. The quantity of exchangeable cations (in meq/kg dry soil) is defined as the cation exchange capacity (CEC).

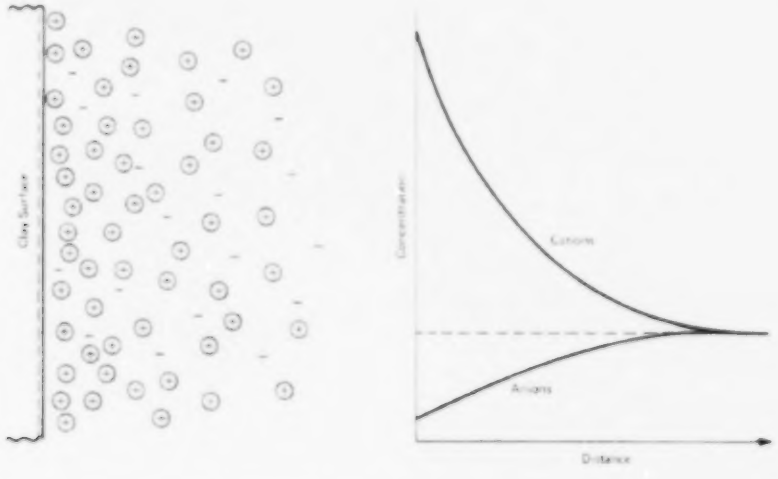


Figure 4.20 - Distribution of ions near clay surface.

Exchangeable cations are available to plants (for example through exchange with H^+ liberated by the roots). Exchange reactions are also responsible for the retention of introduced cations into the soil solution. In this way the CEC gives the soil a buffering capacity, which may slow down the leaching of nutrient cations and positively charged pollutants. CEC is usually dominated by the more abundant cations: Ca, Mg, Na, K, and Al; thus: CEC ≈ 2[Ca] + 2[Mg] + [K] + [Na] + 3[Al] where [M] is the meq per unit mass of exchanger for exchangeable ion M.

The most popular equations describing cation exchange are due to Vanselow (1932), Gaines and Thomas (1953), and Gapon (1933). The Vanselow and Gaines-Thomas conventions differ only in that Vanselow is expressed in mole fractions and Gaines-Thomas is expressed in charge fractions (equivalents). The Gapon convention, in common with the Gaines-Thomas convention, is also expressed in charge fractions.

Because cation exchange is a relatively fast kinetic process, it can modify the chemical composition of both infiltrating water and clays in the solid phase. The exchange reaction of cations M and N (with a charge of m+ and n+, respectively), may be represented using the Gapon convention as:

$$\text{Adsorbed-}N_m + nM^{m+} \Leftrightarrow \text{Adsorbed-}M_n + mN^{n+}$$

Mathematically this reaction has been described by the Gapon equation:

$$\{ \text{Adsorbed(M)} / \text{Adsorbed(N)} \} = K_{NM_G} \times \{ (M^{m+})^{1/m} / (N^{n+})^{1/n} \}$$

with the left-hand side being the ratio of adsorbed M over N (both in meq per mass unit exchanger). The right-hand side contains the reduced activity ratio (where the cation activities are raised to a power equal to the reciprocal of their valence). K_{NM_G} in this equation represents the *Gapon selectivity constant*, which should be constant over a wide range of conditions.

The exchange reaction of cations M and N (with a charge of m+ and n+, respectively), may also be represented using the Gaines-Thomas convention as:

$$m\text{Adsorbed-}N + nM^{m+} \Leftrightarrow n\text{Adsorbed-}M + mN^{n+}$$

The Gaines-Thomas convention leads to the equation:

$$\{ \text{Adsorbed(M)}^n / \text{Adsorbed(N)}^m \} = K_{NM_{GT}} \times \{ (M^{m+})^n / (N^{n+})^m \}$$

Here Adsorbed(M) and Adsorbed(N) are adsorbed amounts of M^{m+} and N^{n+} ions in meq per mass unit exchanger. The solution concentrations on the right hand side of the equation are the ion activities and $K_{NM_{GTi}}$ in this equation represents the *Gaines-Thomas selectivity constant.*

All three exchange-equations (Vanselow, Gapon, Gaines-Thomas) were developed for a constant capacity (permanent charge) exchanger. This implies that if the change in cation exchange complex composition is small compared to the total store of exchangeable cations (which is generally the case, particularly in the short run) the adsorbed ion ratio $\text{Adsorbed(N)}^m / \text{Adsorbed(M)}^n$ remains constant and hence the solution ratio $(N^{n+})^m/(M^{m+})^n$ also remains constant.

The selectivity constant differs from unity, because small size (hydrated) ions are generally preferred over large ones (higher K_{NM}), due to their closer distance of approach to the charged surface. The relative preferences (strength of retention) of the most common cations, for mineral surfaces, are summarized by the Lytropic Series:

$$Al^{3+} > Ca^{2+} > Mg^{2+} > K^{+} > Na^{+}$$

The surface structure of the exchanger (clay surface) may also affect the selectivity constant. Deviations from Lytropic series occur if specific chemical affinity occurs for a particular ion-exchanger pair.

UNSATCHEM uses the Gapon selectivity constants for Ca/Mg, Ca/Na, and Ca/K (Simunek et. al. 1996). The specific Gapon constants are defined as follows:

$$K_{CaMg} = \{ \text{Absorbed(Ca)} / \text{Absorbed(Mg)} \} \times ([Mg]^{1/2} / [Ca]^{1/2})$$

$$K_{CaNa} = \{ \text{Absorbed(Ca)} / \text{Absorbed(Na)} \} \times ([Na] / [Ca]^{1/2})$$

$$K_{CaK} = \{ \text{Absorbed(Ca)} / \text{Absorbed(K)} \} \times ([K] / [Ca]^{1/2})$$

where [M] denotes the equivalent concentration in the solution phase and Absorbed(M) denotes concentration in the solid phase.

VS2DTI uses the Gaines-Thomas selectivity coefficients where the constants for Ca/Mg, Ca/Na, Ca/K are defined as:

$$K_{CaMg} = \{ \text{Absorbed(Ca)}^2 / \text{Absorbed(Mg)}^2 \} \times ([Mg]^2 / [Ca]^2)$$

$$K_{CaNa} = \{ \text{Absorbed(Ca)} / \text{Absorbed(Na)}^2 \} \times ([Na]^2 / [Ca])$$

$$K_{CaK} = \{ \text{Absorbed(Ca)} / \text{Absorbed(K)}^2 \} \times ([K]^2 / [Ca])$$

Table 4.13 gives typical values for Gaines-Thomas and Gapon selectivity coefficients gathered from a brief review the literature.

Table 4.13 - Gaines-Thomas and Gapon selectivity coefficients.

Selectivity Coefficient	Ca-Mg	Ca-Na	Ca-K
Gaines-Thomas	1.1 – 1.9	5.0 – 13	0.03 – 0.07
Gapon	1.0 – 1.4	2.2 – 3.6	0.15 – 0.25

PHREEQC and MINTEQ Manuals
Bond and Phillips, 1990
Cernik *et al*, 1994
Schwiech and Sardin, 1981
Valocchi, 1981
Vulava *et al*, 1999

4.3.1 UNSATCHEM Cation Exchange

Reactive transport (cation exchange) modelling was completed using UNSATCHEM to simulate exchange reactions where solutions with high concentrations of Na^+ would be infiltrating into the groundwater system.

A 1D column simulation was completed for the coarse-fine-coarse soil column with an initial groundwater TDS composition of about 1 kg/m^3. The infiltrating solution had a

concentration of 30 kg/m^3. Gapon selectivity coefficients used for Ca-Mg, Ca-Na and Ca-K were 1.2, 2.9 and 0.2, respectively.

UNSATCHEM allows multicomponent cation-exchange models and calculates sodium absorption ratios (SAR) defined as SAR= [Na+] / { ([Ca2+] + [Mg2+]) / 2}$^{1/2}$. Figure 4.21 illustrates the sodium adsorption ration (SAR) profiles with time.

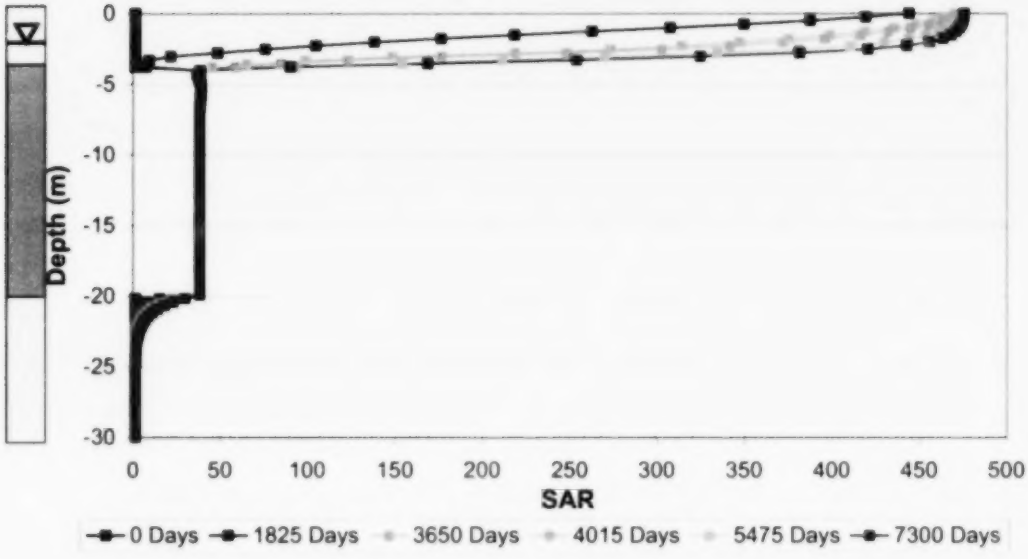


Figure 4.21 - SAR profiles for an infiltrating solution of 30 kg/m^3.

The initial SAR appears to be reasonable given the generic geology of sands and tills and the composition assumed for ambient groundwater. When the contaminant solution with a high ionic strength enters the column with infiltrating groundwater, the SAR values increase to about 500 (consistent with the composition of the salt water). UNSATCHEM was designed to examine the role of major solute species in and below the root zone in terms of irrigation, fertilization and surface and groundwater management. The extreme salinities generated by salt wastes may be outside the intended range of application of the model. Nevertheless, the model does predict the rapid salinization of the upper aquifer and can be used to model the response of the system to addition of Ca-rich infiltration as a result of surface application of gypsum as a soil amendment. Such

simulations may be of greater value for remediation of pipeline breaks and flare pits where Na^+ near-surface concentrations tend to dissipate over time.

4.3.2 VS2DTI Cation Exchange

Reactive transport (cation exchange) modelling was completed using VS2DTI to simulate exchange reactions where solutions with high concentrations of Na+ are infiltrating into the groundwater system.

A 1D simulation was completed for the coarse-fine-coarse soil column with an initial groundwater TDS composition of about 1 kg/m^3. The infiltrating solution had a concentration of 30 kg/m^3. VS2DTI allows a single ion-pair cation-exchange model to be used and saves only the solution chemistry as "total concentration". It was verified that VS2DTI was capable of modelling cation exchange scenarios but results were limited to records of bulk changes in mass balance for ions in solution and on the exchanger.

Any calculation of parameters such as sodium absorption ratios, SAR= [Na+] / { ([Ca2+] + [Mg2+]) / 2}$^{1/2}$, would require source code modifications to VS2DTI to write additional information to output files. Some kind of script could then be written to post process the additional VS2DTI output files. In this regard, UNSATCHEM is significantly more useful for cation-exchange modelling in the present salt-contamination context.

Because VS2DTI has 2D Tier 3 application potential, the cation exchange capabilities may eventually prove to be more valuable than the simple 1-D column model of UNSATCHEM. At the present stage UNSATCHEM is recommended.

5.0 RECOMMENDATIONS

5.1 Responsible Numerical Modelling

Numerical models can be useful tools for understanding contaminant transport at a site. However, the results from the numerical model are dependent upon factors such as input data, mesh design, convergence criteria, and mass balance.

5.1.1 Input Data

Input data should be based primarily on site-specific data. Where site-specific data cannot be obtained, it may be adequate to input data based on parameter estimates from the literature. The adequacy of the geologic model, material properties, contaminant transport properties, and groundwater flow system can be evaluated by viewing the model calibration.

Calibration targets can be pre-determined based on generally accepted criteria. Both qualitative and quantitative calibration criteria can be utilized in the calibration process.

The following list constitutes a set of qualitative targets that an "acceptable" model should satisfy:

- Plume shape and extent estimates based on concentration contours;
- Observed downward movement of brine front using concentration contours;
- Observed hydraulic gradients and flow directions;
- Spatial distribution of groundwater highs and lows; and,
- Estimated fluid fluxes in all aquifers.

5.1.2 Mesh Design

A poorly designed mesh can result in both numerical dispersion and numerical oscillation. One indication of numerical problems is the development of unreasonable concentrations (such as concentrations exceeding source concentration). Numerical oscillation and numerical dispersion can be controlled by satisfying mesh size and time step constraints imposed by the Peclet and Courant number criteria.

Satisfying the Peclet number criterion ensures that the elements are small enough to avoid dispersion that occurs because the movement of contaminant from cell-to-cell in the mesh as a result of successive steps in time occurs faster than the physical mixing process. Numerical dispersion is an artefact of the mesh. The smallest distance that the contaminant can travel in one time-step is the distance between adjacent mesh nodes; if the time-step or mesh spacing is too large, numerical dispersion can become the dominant mixing process. A high degree of spatial resolution is required to avoid excessive "artificial" mixing. The Peclet constraint for the grid size requires that:

$$\Delta x \leq 2D_L / v \approx 2\alpha_L$$

where D_L and α_L are respectively the longitudinal dispersion coefficient and longitudinal dispersivity. This requires that the mesh size in the direction of flow is less than 2 x the dispersivity.

Satisfying the Courant number criterion ensures that the distance of advective contaminant transport in a single time step does not exceed one grid block or element length. The Courant constraint for the time-step size requires that:

$$\Delta t \leq \Delta x / v$$

where v is the advective velocity. Remembering $v = - K(\Delta h/\Delta x)/n$ where K is hydraulic conductivity, n is porosity and $\Delta h/\Delta x$ is the hydraulic gradient. It is easy to see that Δt actually has a quadratic rather than linear dependence on Δx. Unfortunately, when a fine grid is used to reduce numerical dispersion, the time step for dispersive transport calculations may become smaller than the ideal time step for advective calculations, because the dispersive step to satisfy the Courant constraint has quadratic dependence on grid size.

Numerical instabilities (oscillations) in the calculation of diffusion/dispersion are eliminated with the Von Neumann condition constraint (really a combination of the Peclet and Courant constraints):

$$\Delta t \leq \Delta x^2 / 3D_L = \Delta x^2 / 3\alpha_L v$$

It is easy to see that at low advective velocities the constraint is readily satisfied but that progressively smaller Δt is required as Δx decreases.

Spatial and temporal discretization of the model domain must be designed carefully to represent a natural system and avoid artifacts created by the numerical dispersion and oscillations in the calculations. Artificial "mixing" or numerical dispersion is the most serious problem encountered in dispersive/diffusive transport modelling of dense brine transport problems (Uwiera, 1998).

Appendix D illustrates the result of a VS2DTI solution where numerical oscillation has occurred.

5.1.3 Convergence Criteria and Mass Balance

Problems with the specification of convergence criteria can often be diagnosed if the mass balance of the model exceeds an acceptable tolerance. Reducing the convergence criteria for head and/or concentration can usually decrease the mass balance error in a particular simulation. Other factors that may affect the mass balance are mesh spacing and time step size. Reducing these values should also lead to an improved mass balance, provided the Peclet, Courant and Von Neumann numerical constraints continue to be honoured.

There are situations when a relatively large mass balance error may not be indicative of solution error. Changing constant head boundary or initial conditions to simulate changes in site configuration may produce large mass balance errors. The model sees this as an instantaneous change in head and accompanying this head change will be an instantaneous change in fluid stored within an element. Since this increase (or decrease) in storage was not accounted for in the previous time step the model treats it as a discrepancy in the total mass balance.

A common occurrence of this apparent discrepancy is on the very first time step of a simulation when there is an inconsistency between change in initial and/or boundary conditions. Such an occurrence is manifested by a large mass balance error for the first time step.

For this reason it is difficult to recommend a mass balance criterion that all simulations must satisfy. In the absence inconsistencies in initial conditions and boundary conditions or abrupt changes in boundary conditions, a mass balance error of less than 5% is a reasonable target.

5.2 Discussion of Recommended Codes

Four of the codes (CHEMFLO, HYDRUS, UNSATCHEM, and VS2DTI) can be readily applied to 1D Tier 2 analysis for the fate/transport of salt. All four codes produced comparable consistent results for the Tier 2 generic scenarios.

SEVIEW (AT 123D, BIOSCREEN and SESOIL) was the only code tested that was designed to predict groundwater recharge from seasonal climatic data. SESOIL is not recommended because of the difficulties encountered in obtaining reasonable estimates of groundwater recharge through tills for the arid western prairie environment. Nevertheless, AT123D can be used to carry out 1D Tier 2 analysis but without SESOIL has no advantages over the other codes and is limited to homogeneous (or equivalent homogeneous) materials.

For the more complex Tier 3 analysis only VS2DTI and HYDRUS-2D were capable of handling axisymmetric problems. Both codes performed consistently on the 2D generic scenarios but VS2DTI proved more flexible in use.

For cation exchange problems only UNSATCHEM and VS2DTI provided a means of calculation. The two codes use different definitions for selectivity coefficients and are difficult to compare head-to-head. UNSATCHEM is the most sophisticated reactive transport model and readily predicts soil quality parameters such as sodium absorption ratio (SAR) and electrical conductivity (EC).

5.2 CHEMFLO

CHEMFLO is likely the simplest of the codes tested. CHEMFLO is a public domain code that is supported by Oklahoma State University (OSU) Oklahoma Agricultural Experiment Station. The version of CHEMFLO used for the tests was CHEMFLO-2000 beta version 2003.02.26 supplied by the author with added functionality prior to public release.

CHEMFLO is an excellent and effective tool for Tier 2 analysis. General knowledge of the stratigraphic section, elevations of potentiometric surfaces, groundwater recharge rate, basic material properties, and basic chemical transport properties are the minimum required parameters to run CHEMFLO.

CHEMFLO's main strength is its ability to provide results for a simple Tier 2 analysis relatively quickly with simple data input requirements. The input parameters are relatively straightforward and well documented and the user interface is intuitive and easy to use. CHEMFLO also has a java-based interface that gives it added flexibility in terms of platform independence.

CHEMFLO's weakness is that it is a 1D column model. The current public release (2002.08.08) of CHEMFLO can only model the saturated zone to 1 m below the water table. A second problem with the current release of CHEMFLO (2002.08.08) is the restrictions it places on the Van Genuchten beta parameter. Both these restrictions are removed in the version tested in this study and the restrictions will not be present in the next public release of the code. CHEMFLO is also limited to simulating a maximum of four materials, however, this should be adequate enough for most simple Tier 2 analysis problems.

An annoyance associated with CHEMFLO is that it does not save the input data between runs. Printing the screen to the clipboard and saving it in a word processing program such as MS-Word can solve this problem relatively easily, but the data must be re-entered every time the program is executed rather than read from a file.

Although the current release of CHEMFLO (2002.08.08) has limitations, the author provided a beta version of CHEMFLO (2003.02.26) to MDH that corrected the limitation of the Van Genuchten beta parameter and allowed for a larger saturated zone to be modelled. The author expected that the new public release (complete with documentation) will be available in March, 2003, however, no definite time was given for the release date.

CHEMFLO was verified against analytical solutions and other numerical codes as part of the evaluation process and appears to produce accurate consistent results. The code is reliable, well documented, easy to use, in the public domain and supported by a

reputable technical institution. With a java-based interface, it is also has the added advantage of platform-independence.

The revised version of CHEMFLO to be released after March 2003 is recommended as first choice for Tier 2 analysis.

5.3 HYDRUS

HYDRUS-2D was one of two 2D codes tested in the group of five codes selected for detailed review in Phase II. HYDRUS is a proprietary code that is supported by the United States Salinity Laboratory (USSL) and distributed by the International Groundwater Modelling Centre (IGWMC) at the Colorado School of Mines. The version tested was HYDRUS-2D version 2.007.

HYDRUS is an effective tool for Tier 2 analysis and can be applied to most Tier 3 problems. General knowledge of the stratigraphic section, elevations of potentiometric surfaces, groundwater recharge rate, basic material properties, and basic chemical transport properties are the minimum required parameters to run HYDRUS for 1D column analysis and for 2D axisymmetric problems.

The main strength of HYDRUS is its ability to provide results for both simple Tier 2 analysis and more complex 2D axisymmetric analysis for Tier 3 assessment. HYDRUS automatically adjusts the time step to ensure that the Courant criterion is satisfied and reports the critical grid Peclet number. This is a valuable feature for ensuring the quality of results.

The main disadvantages of HYDRUS are its inability to simulate an irregular (non-rectangular) geometry without purchasing an additional proprietary mesh generator and a large number of "built-in" undocumented restrictions.

1. With the "basic" mesh generator supplied with HYDRUS, specifying a mesh with variable spacing is tedious. When the mesh is changed material property boundaries and boundary conditions must be re-specified. The version of HYDRUS tested (2.007) crashes if the mesh spacing is expanded using an

expansion factor above a critical value (but does not warn the user of such a restriction).

2. The HYDRUS solver stability also appears to be somewhat sensitive to mesh spacing. Again the program crashes without prior warning of a restriction and the user may need to increase or decrease the mesh size (and must consequently re-specify all material boundaries and flow and transport boundary conditions).

3. For the generic axisymmetric scenario with a pipe break, it was necessary to use an "internal" nodal flux boundary condition with a specified source concentration. Such boundary conditions are poorly documented in HYDRUS and there is an unspecified maximum flux rate that can be applied. Again the program crashes without warning if this threshold value is exceeded.

4. HYDRUS cannot simulate multiple recharge periods with different boundary conditions within the same simulation. However, the package does allow the user to import concentrations and pressure heads from previous simulations. Unfortunately, there is an unspecified restriction on the number of nodal concentration values that can be imported in an ASCII file (although no such restriction applies to heads or to concentrations if the file is saved in binary format).

HYDRUS-2D is certainly adequate to use for Tier 2 analysis but has little to offer over CHEMFLO, UNSATCHEM and VS2DTI in this role. HYDRUS-1D can also perform the same function (but was not tested in this phase of the study). Over all, HYDRUS is a well-written and reliable numerical code that produced accurate results on all verification problems. It's major fault is a poor user interface that fails to protect the user from predictable parameter limitations and input-output restrictions.

Although the HYDRUS-2D code is fundamentally sound and has many excellent features, the limitations of the program are significant enough to not recommended its use for Tier 3 analysis.

5.4 SEVIEW

SEVIEW is a proprietary "GUI wrapper" around the public-domain BIOSCREEN, SESOIL and AT123D codes. The GUI generates input for the AT123D contaminant

transport code using SESOIL. The version of the package tested was SEVIEW version 6.0.

Detailed knowledge of the seasonal climatic data and chemical properties are required to run SESOIL. General knowledge of the stratigraphic section, groundwater flow conditions, groundwater recharge rate and basic soil properties are the minimum required parameters to run Tier 2 1D column problems in SEVIEW.

SEVIEW's main strength is the ability of the SESOIL model to predict groundwater recharge from measured monthly or daily climatic data. The performance of SESOIL as a tool to generate groundwater recharge from a water balance was disappointing.

SEVIEW's main weakness is SESOIL's requirement of extensive climatic and chemical input data. Using "raw" monthly climate data for sites in the western Canadian prairies SESOIL was not able to generate credible groundwater recharge rates for fine-grained, low-permeability soils (despite numerous attempts). SEVIEW allows up to four heterogeneous soil-layers but generates a single "equivalent" homogeneous material for the SESOIL analysis. Only a homogeneous material can be input into AT123D. The inability of SEVIEW to simulate truly heterogeneous soil systems limits the number of sites in Alberta where the code could be applied (even for Tier 2 analysis). SEVIEW appears to be designed for organic contaminants at low concentrations in moderate to high permeability agricultural soils.

Without SESOIL, AT123D has many limitations and no advantages over CHEMFLO, HYDRUS, UNSATCHEM and VS2DTI. For this reason, systematic further testing of AT123D was discontinued.

SEVIEW is not recommended as a suitable code for screening of salt contaminated sites in Alberta.

5.5 UNSATCHEM

UNSATCHEM is a public domain code that was written by the United States Salinity Laboratory and is receiving limited support. It has been superseded by HYDRUS-1D (which was not tested). The version of UNSATCHEM used for the tests was UNSATCHEM version 2.0 with a compilation date in 1996.

General knowledge of the stratigraphic section, elevations of potentiometric surfaces, groundwater recharge rate, basic material properties, and basic chemical transport properties are the minimum required parameters to run UNSATCHEM.

UNSATCHEM is a reliable and relatively easy-to-use 1D code for Tier 2 analysis but is not the first-choice for such applications.

UNSATCHEM's main advantage lies in it ability to simulate cation ion-exchange reactions as a component of simple Tier 2 1D column problems. The input parameters are relatively straightforward and reasonably well documented (although some sign conventions are poorly explained). The user interface is less than intuitive but relatively easy-to-use once familiarity has been gained.

UNSATCHEM's main disadvantages are associated with the specification of boundary conditions. A constant flux boundary must be applied as negative for movement of water into the column and positive for movement of water out of the column. This flux boundary condition is recommended for use over the atmospheric flux boundary condition because UNSATCHEM appears to treat the concentration flux boundary as a constant concentration boundary when an atmospheric flux boundary condition is applied at the surface.

Another disadvantage of UNSATCHEM is its inability to import pressure head or concentration data from previous runs or to use multiple recharge periods with a constant flux boundary. In order to complete the 1D simulations, MDH had to manually input the output data from one run as the initial condition for a second run to simulate the removal of a source. This inflexibility limits the usefulness of UNSATCHEM.

A major concern with UNSATCHEM is the lack of further development and the limited nature of the support for the code. HYDRUS-1D is the proprietary replacement for the public domain UNSATCHEM code but lacks the sophistication of UNSATCHEM for reactive transport modelling.

In order to use the advanced reactive transport capabilities of UNSATCHEM, addition information on the chemical parameters (particularly soil chemistry and mineralogy, cation exchange capacity, and ambient groundwater and pore-water chemistry) is required. Such data is generally collected as part of Tier 3 assessments. The reactive

transport capabilities of UNSATCHEM can provide a means of quantifying the effects of applying gypsum amendment to the surface soils in the vicinity of remediated pipe breaks and flare pit sites.

UNSATCHEM was verified against analytical solutions and other numerical codes as part of the evaluation process and appears to produce accurate consistent results. The code is reliable, well documented, easy-to-use, and in the public domain.

UNSATCHEM is recommended for use in Tier 3 assessment where simulation of cation exchange processes is a requirement.

5.6 VS2DTI

VS2DTI is the second of two 2D codes tested in Phase 2 of the project. VS2DTI is a public domain code supported by the United States Geological Survey (USGS). The version tested was VS2DTI version 1.1.

VS2DTI is an excellent code for both Tier 2 (1D columns) and Tier 3 (2D axisymmetric) analysis of salt transport (at low concentration). General knowledge of the stratigraphic section, elevations of potentiometric surfaces, groundwater recharge rate, basic material properties, and basic chemical transport properties are the minimum required parameters to run VS2DTI for 1D column analysis and for 2D axisymmetric problems.

VS2DTI's main advantage lies in its extreme flexibility (it was the only code to simulate every one of the generic scenarios without significant difficulty). VS2DTI has a good user-friendly interface although some of the important time saving features are not obvious to the first-time user. VS2DTI separates the definition of the model domain, material properties and boundary conditions from the generation of a mesh. This means that a problem can be re-meshed in seconds and identical problems are readily run on multiple meshes. This is a major advantage when checking the validity of results. VS2DTI also allows multiple recharge periods to be specified with different boundary conditions and numerical time-stepping parameters. Again, this provides for easy checking and adds to flexibility. VS2DTI has the ability to model cation exchange reactions although the post-processing options in respect of this feature are minimal.

VS2DTI's main disadvantage is that solutions can be extremely sensitive to mesh discretization and sometimes, initial conditions. Unlike HYDRUS, VS2DTI does not automatically adjust the time step to satisfy the Courant condition and does not automatically output the grid Peclet number. Extreme care is needed with mesh design and the specification of initial conditions to ensure that "valid" results are obtained. VS2DTI does report mass balance errors to the screen during simulation runs but their interpretation requires technical knowledge and experience.

Although VS2DTI allows the user to input the number of iterations for convergence of transport steps, the program ignores the parameters input by the user if a threshold value of 200 is exceeded. Editing and re-compiling the source code could easily fix this, but the interface should warn the user of the limitation. Another disadvantage of VS2DTI is the inability to cut cross-sections of data and to view graphs of concentration or head versus time or distance in the postprocessor. The CHEMFLO, HYDRUS and UNSATCHEM post-processing capabilities are better in this area.

VS2DTI models cation exchange using the Gaines-Thomas convention for selectivity coefficients. Unfortunately, the program appears to save only rudimentary information about reactive chemical processes. It is not possible to plot cation ratios either against time or spatially for either the solution or the exchanger. Source code modifications would be necessary to implement such a feature.

VS2DTI was verified against analytical solutions and other numerical codes as part of the evaluation process and appears to produce accurate consistent results. The code is reliable, well documented, easy to use, in the public domain and supported by a reputable technical institution. With a java-based interface, it is also has the added advantage of platform-independence

VS2DTI is recommended for application to both 1D column (Tier 2) and 2D axisymmetric (Tier 3) scenarios.

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7.0 CLOSURE

We trust that this report meets all your present requirements. Should you have any questions or comments please contact us. We look forward to discussing this report further with you in the near future.

Respectfully submitted,
MDH Engineered Solutions

Association of Professional Engineers,
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APPENDIX A

DETAILED INPUT DATA

Table A2 Complete input data requirements for CHEMFLO, HYDRUS, UNSATCHEM, VS2DTI

This table identifies what parameters need to be input with each model. If the cell says 'Yes' then the variable must be entered into the model. If the cell says 'No' then there is no option to enter the variable into the model. If the cells says 'Opt' then the variable can be input into the model, but nothing needs to be input into the model if it is not clicked on in the model.

	Must be measured/provided
	Must be estimated
	Not needed/Default

#	Variable	Unit	Program				
			CHEMFLO	M-VIEW	UNSATCHEM	HYDRUS2D	VS2DTI
	SOLUTE PROPERTIES						
1	Solubility	mg/L	No	Yes	No	No	No
2	Molecular weight	g/mol	No	Yes	No	No	No
3	Henry's constant	-	No	Yes	No	Yes	Opt
4	Chemical reference	-	No	Yes	No	No	No
	BOUNDARY CONDITIONS						
5	Hydraulic Surface Boundary						
	Constant flux	L/T	Opt	No	Opt	Opt	Opt
	Variable flux	L/T	No	Opt	Opt	Opt	Opt
	Constant head	L	Opt	No	Opt	Opt	Opt
	Atmospheric BC with surface layer	L/T	No	No	Opt	Opt	No
	Atmospheric BC with surface runoff	L/T	No	No	Opt	No	No
	Surface runoff	L/T	No	Opt	No	No	Opt
	Seepage face	cm/dt	No	No	Opt	Opt	Opt
6	Hydraulic Base Boundary						
	Constant flux	L/T	Yes	No	Opt	Opt	Opt
	Constant head	L	Yes	No	Opt	Opt	Opt
	Variable flux	L/T	No	No	Opt	Opt	Opt
	Variable head	L	No	No	Opt	Opt	Opt
	Free drainage	-	Opt	No	Opt	Opt	No
	Deep drainage	-	No	No	Opt	Opt	No
61	Concentration Surface Boundary	M/L3					
	Inflow solution	M/L3	Opt	-	Opt	Opt	Opt
	Ambient soil solution	M/L3	Opt	-	Opt	Opt	Opt
62	Concentration Base Boundary	-					
	Exit solution	M/L3	Opt	-	Opt	Opt	Opt
	Exit flux	M/T	No	-	Opt	Opt	Opt
	Convective flow	L/T	Opt	-	No	No	No
	Zero gradient	-	No	-	Opt	No	No
	Variable flux	M/T	No	-	No	Opt	No
	Zero solute flux	-	No	-	No	Opt	Opt
	CONCENTRATION VALUES						
63	Concentrations						
	Location of maximum concentration	M/L3	Yes	Yes	Yes	Yes	Yes
	Location of zero concentration	M/L3	Yes	Yes	Yes	Yes	Yes
	Conceptual Rate Groundwater plume will move	M/L3	Yes	Yes	Yes	Yes	Yes
#	Additional 2-D parameter	Unit	Program				
			CHEMFLO	M-VIEW	UNSATCHEM	HYDRUS2D	VS2DTI
64	Degree of anisotropy	-	No	Yes	No	Yes	Yes

#	Variable	Unit	Program				
			CHEMFLO	M-VIEW	UNSATCHEM	HYDRUS2D	VS2DTI
	SOIL PROPERTIES						
26	SWCC	-					
	Qm (soil water retention function	-	No	No	Yes	Opt	No
	Qs (soil water retention function	-	No	No	Yes	Opt	No
	Alpha parameter	1/L	Yes	No	Yes	Yes	Yes
	Beta or n parameter	-	Yes	No	Yes	Yes	Yes
27	Soil pore dissconnectivess	-	No	Yes	No	No	No
28	Specific storage	-	No	No	No	No	Yes
	SOLUTE PROPERTIES						
29	Dispersion coefficient	L2/T					
30	Longitudinal dispersivity	L	Yes	Yes	Yes	Yes	Yes
31	Transverse dispersivity	L	No	Yes	No	Yes	Yes
32	Diffusion coefficient (ions in porous medium	L2/T	Yes	Yes	Yes	Yes	Yes
33	K_d						
	Uniform soil water partition coefficient	L3/M	Yes	Yes	No	No	K_d
	Freundlich adsorption isotherm		No	Yes	No	No	K_d
	Adsorption isotherm coefficient to		No	No	No	Yes	No
34	Ion Exchange						
	Kn, Gaines-Thomas ion-exchange selectivity coefficient	-	No	No	No	No	Opt
	Kg, Gapon ion-exchange selectivity coefficient	-	No	No	Yes	No	No
35	Solubility in water	M/L3	No	Yes	No	No	No
36	Molecular weight	g/mol	No	Yes	No	No	No
37	Henry's constant	-	No	Yes	No	Yes	Opt
38	Chemical reference	-	No	Yes	No	No	No
	BOUNDARY CONDITIONS						
39	Hydraulic Surface Boundary						
	Constant flux	L/T	Opt	No	Opt	Opt	Opt
	Variable flux	L/T	No	Opt	Opt	Opt	Opt
	Constant head	L	Opt	No	Opt	Opt	Opt
	Atmospheric BC with surface layer	L/T	No	No	Opt	Opt	No
	Atmospheric BC with surface runoff	L/T	No	No	Opt	No	No
	Surface runoff	L/T	No	Opt	No	No	Opt
	Seepage face	cm/dt	No	No	Opt	Opt	Opt
40	Hydraulic Base Boundary						
	Constant flux	L/T	Yes	No	Opt	Opt	Opt
	Constant head	L	Yes	No	Opt	Opt	Opt
	Variable flux	L/T	No	No	Opt	Opt	Opt
	Variable head	L	No	No	Opt	Opt	Opt
	Free drainage	-	Opt	No	Opt	Opt	No
	Deep drainage	-	No	No	Opt	Opt	No
41	Concentration Surface Boundary	M/L3					
	Inflow solution	M/L3	Opt	-	Opt	Opt	Opt
	Ambient soil solution	M/L3	Opt	-	Opt	Opt	Opt
42	Concentration Base Boundary	-					
	Exit solution	M/L3	Opt	-	Opt	Opt	Opt
	Exit flux	M/T	No	-	Opt	Opt	Opt
	Convective flow	L/T	Opt	-	No	No	No
	Zero gradient	-	No	-	Opt	No	No
	Variable flux	M/T	No	-	No	Opt	No
	Zero solute flux	-	No	-	No	Opt	Opt
	CONCENTRATION VALUES						
43	Concentrations						
	Location of maximum concentration	M/L3	Yes	Yes	Yes	Yes	Yes
	Location of zero concentration	M/L3	Yes	Yes	Yes	Yes	Yes
	Conceptual Rate Groundwater plume will move	M/L3	Yes	Yes	Yes	Yes	Yes
#	Additional 2-D parameter	Unit	Program				
			CHEMFLO	M-VIEW	UNSATCHEM	HYDRUS2D	VS2DTI
44	Degree of anisotropy	-	No	Yes	No	Yes	Yes

Table A3 Complete input data requirements for CHEMFLO, HYDRUS, UNSATCHEM, VS2DTI

This table identifies what parameters need to be input with each model. If the cell says **'Yes'** then the variable must be entered into the model. If the cell says **'No'** then there is no option to enter the variable into the model. If the cell's say **'Opt'** then the variable can be input into the model, but nothing needs to be input into the model if it is not clicked on in the model.

[redacted] Must be measured/provided
[redacted] Must be estimated
[redacted] Not needed/Default

#	Variable	Unit	Program				
			CHEMFLO	REVEW	UNSATCHEM	HYDRUS2D	VS2DTI
	SOIL PROPERTIES						
45	[redacted]						
	SOLUTE PROPERTIES						
46	[redacted]						
47							
48							
49							
50							
51							
52							
53							
54							
55							
56							
57							
58							
59							
60							
61							
62							
63							
64							
65							
	ROOT GROWTH PROPERTIES						
66	[redacted]						
67							
68							
69							
70							
71							
72							
	ROOT UPTAKE PROPERTIES						
73	[redacted]						
74							
75							
76							
77							
78							
79							
80							
81							
82							
83							
84							
85							
86							
87							
88							
89							
90							
91							
92							
	CARBON DIOXIDE TRANSPORT						
93	[redacted]						
	HEAT TRANSPORT						
94	[redacted]						

#	Variable	Unit	Program				
	Dependence in soil water retention curve		No	No	Yes	Opt	No
	Adsorption						
	Adsorption isotherm coefficient -		No	No	No	Yes	No
	Adsorption isotherm exponent [		No	No	No	Yes	No
	Organic carbon fraction		Yes	Yes	No	Opt	No
	Dissolved organic carbon		No	No	Opt	No	No
	Reduction in Kd due to solution chemistry		No	No	Opt	No	No
	Concentration dependence for water flow parameters		No	No	No	Opt	No
	Ion exchange capacity		No	Yes	Opt	Yes	No
	Decay coefficients						
	first order decay coefficient (liquid)		Yes	Yes	No	Yes	Yes
	first order decay coefficient (solid)		Yes	Yes	No	Yes	No
	first order decay coefficient (gas)		No	No	No	Yes	No
	first order decay coefficient for chain reacts		No	No	No	Yes	No
	first order decay coefficient for chain reacts		No	No	No	Yes	No
	first order decay coefficient for chain reacts		No	No	No	Yes	No
	Production coefficients						
	zero order production coefficient (gas)		No	No	Opt	Yes	No
	zero order production coefficient (solid)		Yes	No	No	Yes	No
	Alpha (1st order rate transfer of non-equil mtrx		No	No	No	Yes	No
	Fract (fraction of type1 sorption sites		No	No	No	Yes	No
	Mobwat (mobile water content non-equil		No	No	No	Yes	No
	Canopy surface area		No	No	Yes	No	No
	Snowpack surface area		No	No	Yes	No	No
	Specific kinetic precipitation/dissolution		No	No	Opt	No	No
	Base hydrolysis rate		No	Yes	No	No	No
	Neutral hydrolysis rate constant		No	Yes	No	No	No
	Acid hydrolysis rate constant		No	Yes	No	No	No
	Ligand dissociation constant		No	Yes	No	No	No
	Active Ligand/metals chemtox		No	Yes	No	No	No
	Antioxidant wt. Ligand		No	Yes	No	No	No
	Root growth		No	No	Opt	No	No
	Initial root growth bmx		No	No	Opt	No	No
	Harvest bmx		No	No	Opt	No	No
	Initial rooting depth		No	No	Opt	No	No
	Max rooting depth		No	No	Opt	No	No
	Lime root data		No	No	Opt	No	No
	Depth root data		No	No	Opt	No	No
	Root water uptake		No	No	Opt	Opt	Opt
	Uptake flux		No	No	Opt	No	No
	A0		No	No	Opt	No	No
	A50		No	No	Opt	No	No
	Alpha		No	No	Opt	No	No
	Alpha0		No	No	Opt	No	No
	A3		No	No	No	Opt	No
	Actgt		No	No	No	Opt	No
	Alpl		No	No	No	Opt	No
	A2L		No	No	No	Opt	No
	A3		No	No	No	Opt	No
	Alim		No	No	No	Opt	No
	A2L		No	No	No	Opt	No
	Potential evaporation		No	No	No	No	Opt
	Pressure potential of atmosphere		No	No	No	No	Opt
	Potential transpiration		No	No	No	No	Opt
	Rooting depth		No	No	No	No	Opt
	Activity at root base		No	No	No	No	Opt
	Activity at root top		No	No	No	No	Opt
	Pressure head in root		No	No	No	No	Opt
	Many variables		No	No	Opt	No	No
	Many variables		No	No	Opt	Opt	Opt

Table A1 Detailed input data for CHEMFLO, HYDRUS, UNSATCHEM, VS2DTI

Variable	Unit	Program			
		CHEMFLO	HYDRUS	UNSATCHEM	VS2DTI
SOIL PROPERTIES:					
Moisture Content					
saturated moisture content (θ_s) - Coarse Material	--	0.25	0.25	0.25	0.25
residual moisture content (θ_r) - Coarse Material	--	0.05	0.05	0.05	0.05
saturated moisture content (θ_s) - Fine Material	--	0.38	0.38	0.38	0.38
residual moisture content (θ_r) - Fine Material	--	0.3	0.3	0.3	0.3
parameter of the soil retention curve (θ_p)[1]	--	No Option	No Option	(0r)	No Option
parameter of the soil retention curve (θ_m)[1]	--	No Option	No Option	(0s)	No Option
Permeability					
saturated hydraulic conductivity (Ks) - Coarse Material	m/d	8.9	8.9	8.9	8.9
saturated hydraulic conductivity (Ks) - Fine Material	m/d	8.6×10^{-4}	8.6×10^{-4}	8.6×10^{-4}	8.6×10^{-4}
unsaturated hydraulic conductivity (Kk)[1] corresponding to (θ_k)[1]	m/d	No Option	No Option	Ks	No Option
relative hydraulic conductivity (Kr)	m/d	No Option	No Option	Ks	No Option
reduction in hydraulic conductivity due to solution chemistry	on/off	No Option	No Option	Turned Off	No Option
SWCC					
Van Genuchten - α parameter - Coarse Material	m^{-1}	12	12	12	12
Van Genuchten - β parameter - Coarse Material	--	2.7	2.7	2.7	2.7
Van Genuchten - α parameter - Coarse Material	m^{-1}	1.5	1.5	1.5	1.5
Van Genuchten - β parameter - Coarse Material	--	1.1	1.1	1.1	1.1
Pore Conductivity Parameter - Coarse Material[2]	--	No Option	0.5	No Option	No Option
Pore Conductivity Parameter - Fine Material[2]	--	No Option	0.5	No Option	No Option
Specific Storage - Coarse Material	m^{-1}	No Option	No Option	No Option	1×10^{-4}
Specific Storage - Fine Material	m^{-1}	No Option	No Option	No Option	1×10^{-4}
Degree of anisotropy - Coarse Material	--	No Option	1	No Option	1
Degree of anisotropy - Fine Material	--	No Option	1	No Option	1
Bulk density - Coarse Material	kg/m^3	1750	1750	1750	1750
Bulk density - Fine Material	kg/m^3	1750	1750	1750	1750
SOLUTE PROPERTIES:					
Dispersion coefficient					
longitudinal dispersivity	m	0.4	0.4	0.4	0.4
transverse dispersivity	m	No Option	0.04	No Option	0.04
Diffusion coefficient (ions in soil)					
diffusion coefficient (Na^+) - coarse soil	m^2/d	2.9×10^{-3}	2.9×10^{-3}	2.9×10^{-3}	2.9×10^{-3}
diffusion coefficient (Na^+) - fine soil	m^2/d	No Option	No Option	4.0×10^{-3}	4.0×10^{-3}
diffusion coefficient (air)	m^2/d	No Option	0	Not Required	No Option
K_d					
uniform soil water partition coefficient	m^3/kg	0	No Option	No Option	Turned Off
Freundlich adsorption isotherm	m^3/kg	No Option	Below	No Option	Turned Off
adsorption isotherm coefficient kd	m^3/kg	No Option	0	No Option	No Option
adsorption isotherm coefficient γ	m^3/kg	No Option	0	No Option	No Option
adsorption isotherm exponent β	--	No Option	1	No Option	No Option
Ion Exchange					
Km: Gaines-Thomas ion-exchange selectivity coefficients (Ca-Na)		No Option	No Option	No	8.5
Km: Gaines-Thomas ion-exchange selectivity coefficients (Ca-Mg)		No Option	No Option	No	1.2
Km: Gaines-Thomas ion-exchange selectivity coefficients (Ca-K)		No Option	No Option	No	0.05
Kg: Gapon ion-exchange selectivity coefficients (Ca-Na)		No Option	No Option	2.9	No Option
Kg: Gapon ion-exchange selectivity coefficients (Ca-Mg)		No Option	No Option	1.2	No Option
Kg: Gapon ion-exchange selectivity coefficients (Ca-K)		No Option	No Option	0.2	No Option
Cation exchange capacity	meq/kg	No Option	No Option	90	90
Calcite surface area	m^2	No Option	No Option	0	No Option
Dolomite surface area	m^2	No Option	No Option	0	No Option
Specify kinetic precipitation/dissolution	on/off	No Option	No Option	Turned Off	No Option
Organic carbon fraction		0	Not Required	Not Required	Not Required
Decay coefficients					
first order decay coefficients	d^{-1}	0	0	No Option	0
first order decay coefficient for chain react's	d^{-1}	No Option	0	No Option	No Option
Production coefficients					
zero order production coefficient(gas)	d^{-1}	No Option	0	Turned off	No Option
zero order production coefficient (solid)	d^{-1}	0	0	No Otpion	No Option
Chemical Non-Equilibrium Parameters					
Fract[3]	--	No Option	1	No Option	No Option
Alpha[4]	d^{-1}	No Option	0	No Option	No Option
Physical Non-Equilibrium Parameters					
Thimob[5]	m^3/m^3	No Option	0	No Option	No Option
Temperature Dependent Parameters					
Henry[6]	--	No Option	0	No Option	Not Required
temperature dependence for water flow parmeters	on/off	No Option	Turned Off	No Option	No Option

(1) Simunek, Suarez, and Sejna (1996) suggest that the hydraulic characteristics contain 9 unknown parameters, θ_r, θ_s, θ_p, θ_m, α, β, K_s, K_p, θ_k. When $\theta_p = \theta_r$, $\theta_m = \theta_s$, and $K_p = K_s$, the soil hydraulic functions reduce to the original expressions of van Genuchten (1980).

(2) Simunek, Sejna and Van Genuchten (1999) suggest that the pore-connectivity parameter (l) in the hydraulic conductivity function was estimated (Mualem, 1976) to be about 0.5 as an average for most soils.

(3) Fract. - Dimensionless fraction [-] of the sorption sites classified as type-1, (i.e., sites subject to instantaneous sorption) when chemical nonequilibrium is simulated, or dimensionless fraction of sorption sites in contact with mobile water when physical nonequilibrium is simulated. Author says default is one if non-equilibrium is not considered.

(4) Alpha - First-order rate transfer coefficient for nonequilibrium sorption when chemical nonequilibrium is simulated, or for exchange between mobile and immobile liquid regions when physical nonequilibrium is simulated.

(5) Thimob - Immobile water content when physical nonequilibrium is simulated.

(6) Henry - Equilibrium distribution constant between liquid and gas phases.

APPENDIX B

1D DETAILED OUTPUT DATA

Figure B1 - Source applied to a coarse-grained soil column for 5 Years.

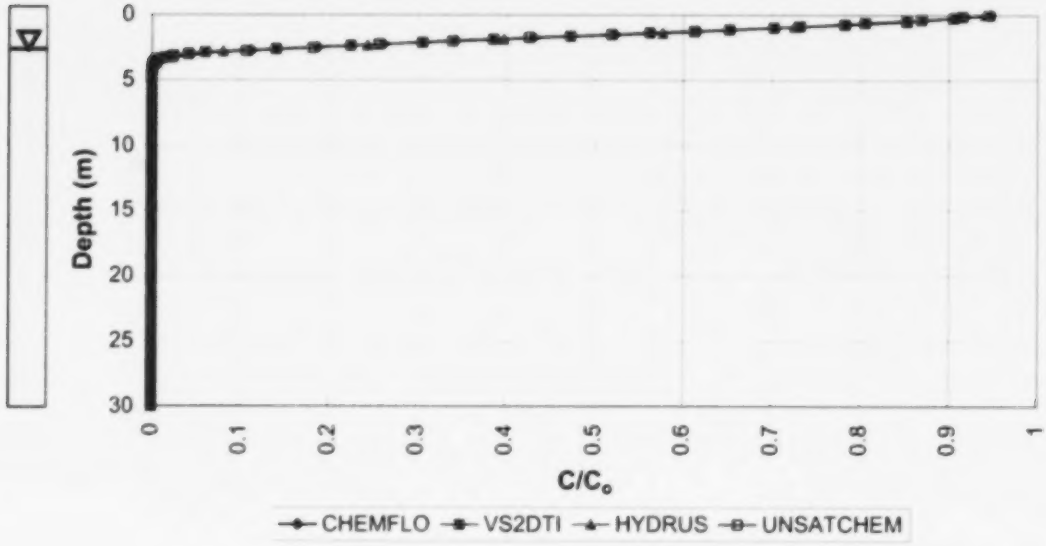


Figure B2 - Source applied for to a coarse-grained soil column 10 years.

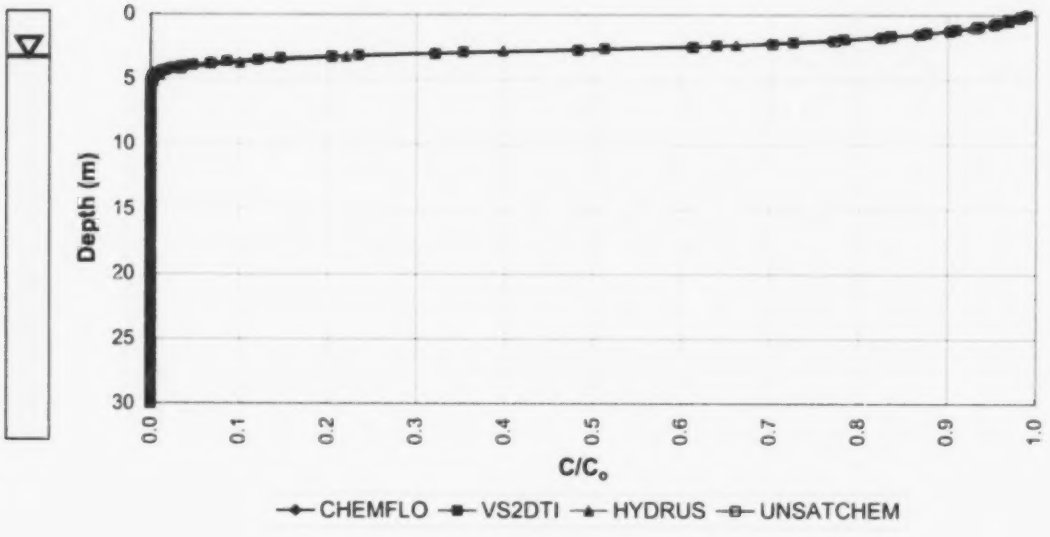


Figure B3 - Source applied to a coarse-grained soil column for 15 years.

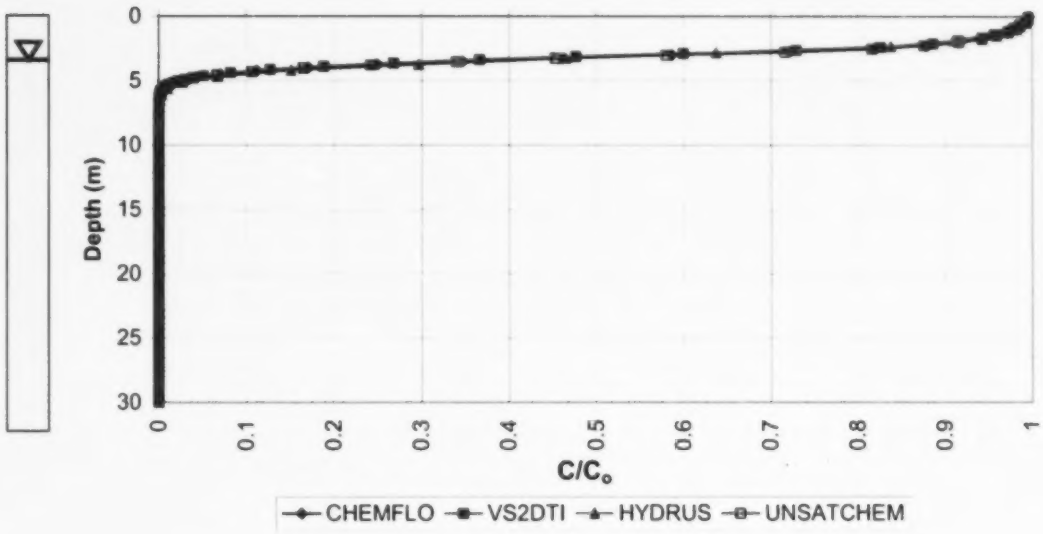


Figure B-4 Source applied to a coarse-grained soil column for 20 years.

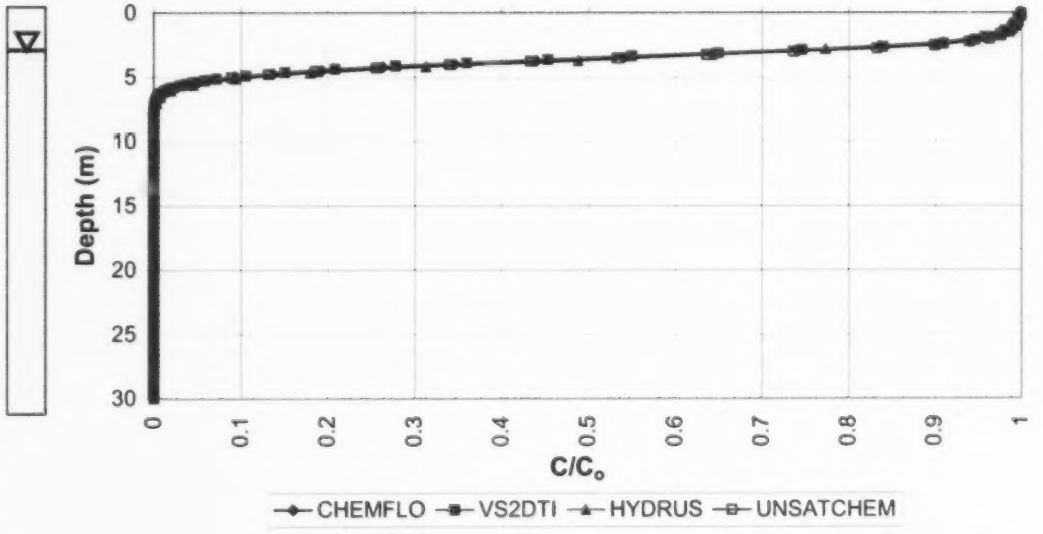


Figure B5 - Source removed from a coarse-grained soil column for 5 years.

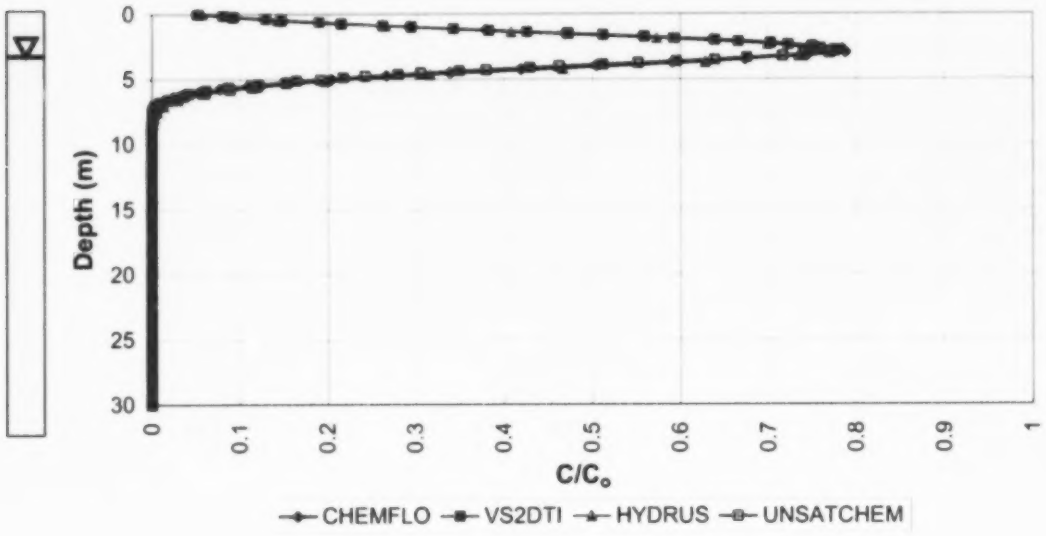


Figure B6 - Source removed from a coarse-grained soil column for 10 years.

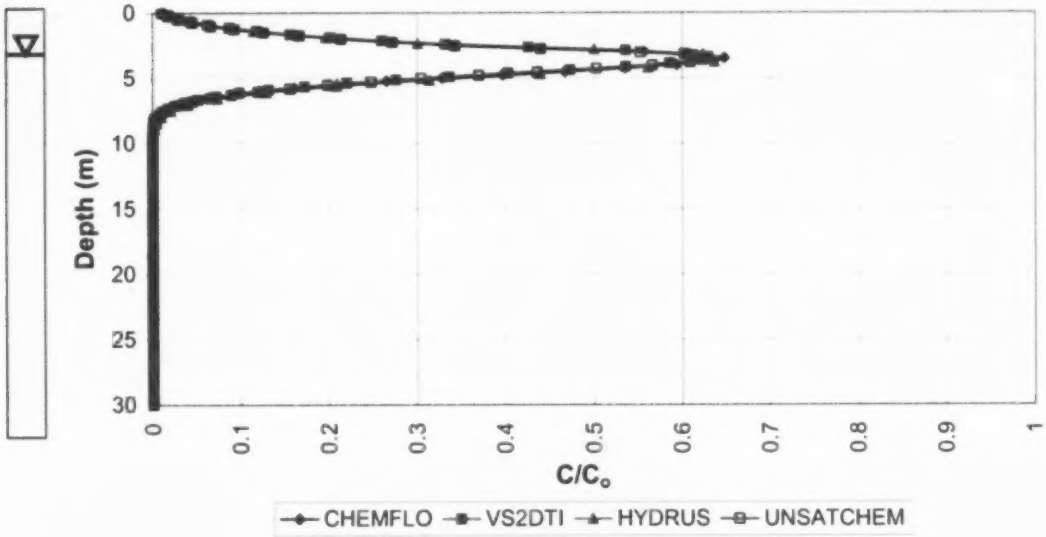


Figure B7 - Source removed from a coarse-grained soil column for 15 years.

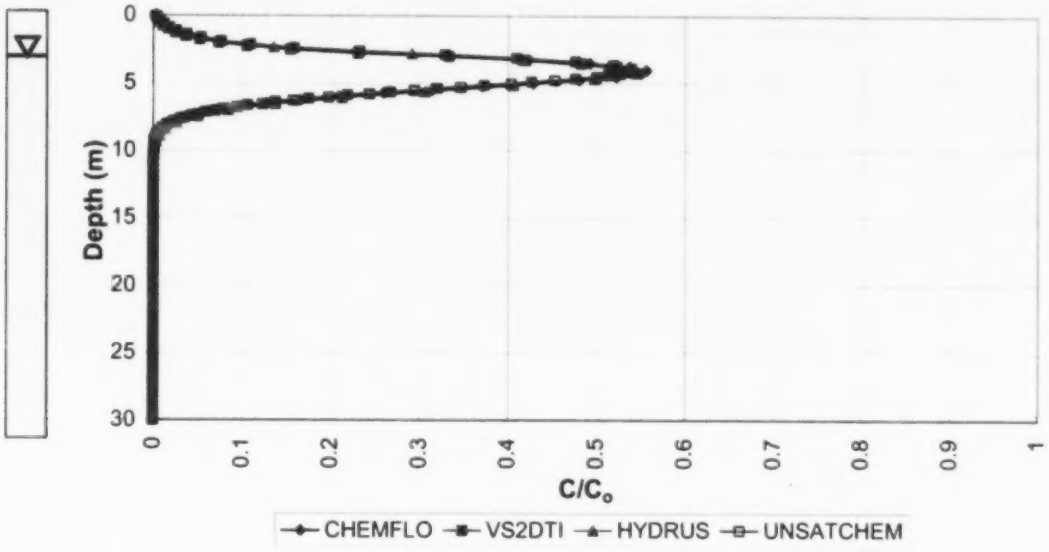


Figure B8 - Source removed from a coarse-grained soil column for 20 years.

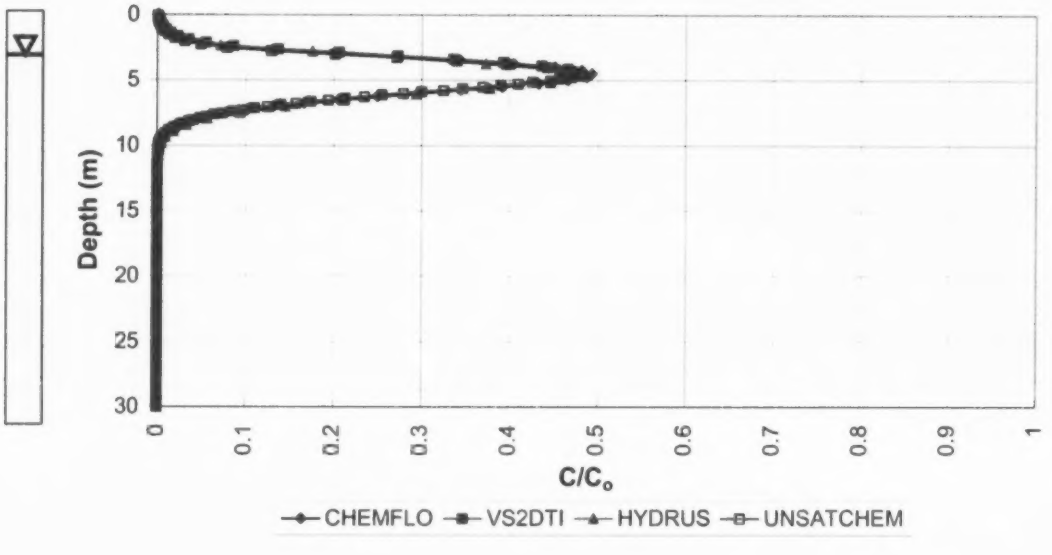


Figure B9 - Source added to a fine-grained soil column for 5 years.

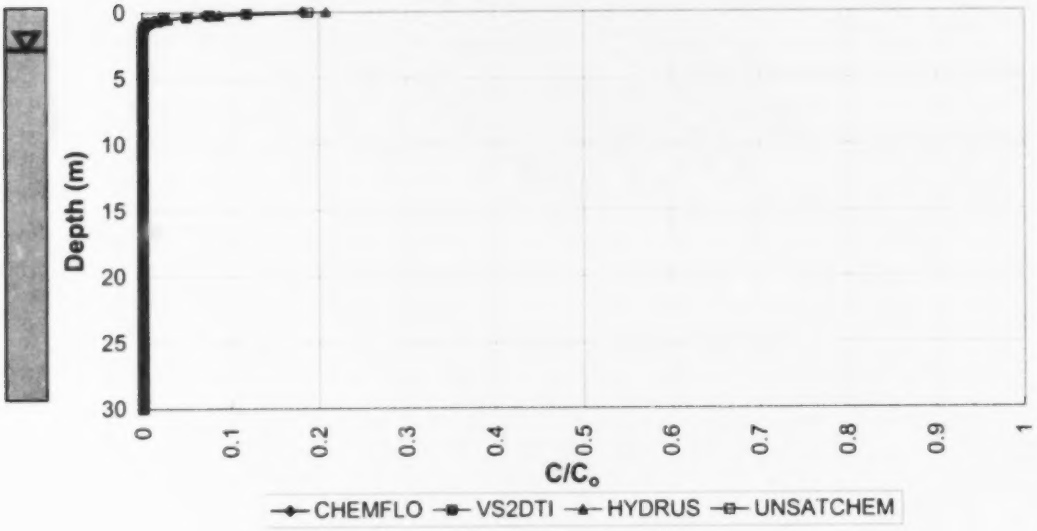


Figure B10 - Source added to a fine-grained soil column for 10 years.

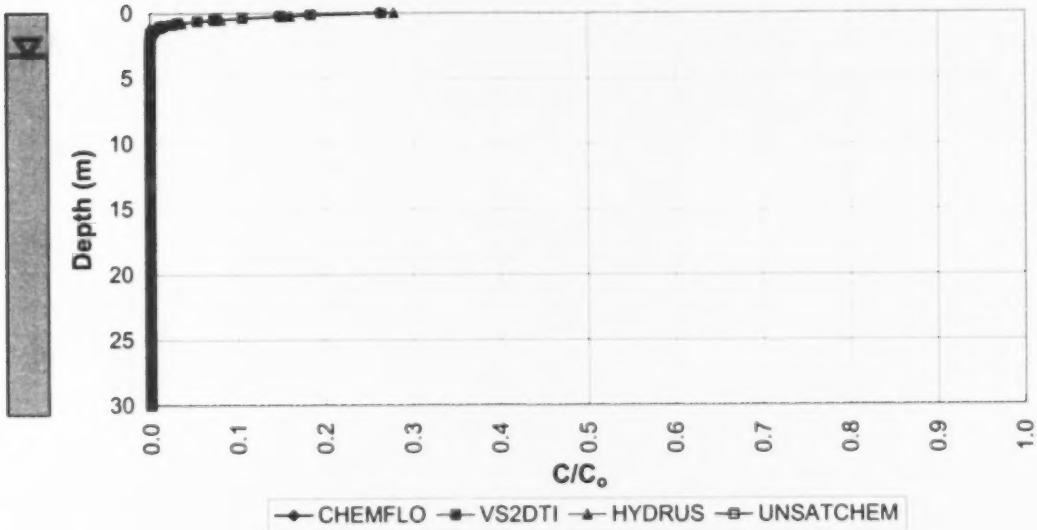


Figure B11 - Source added to a fine-grained soil column for 15 years.

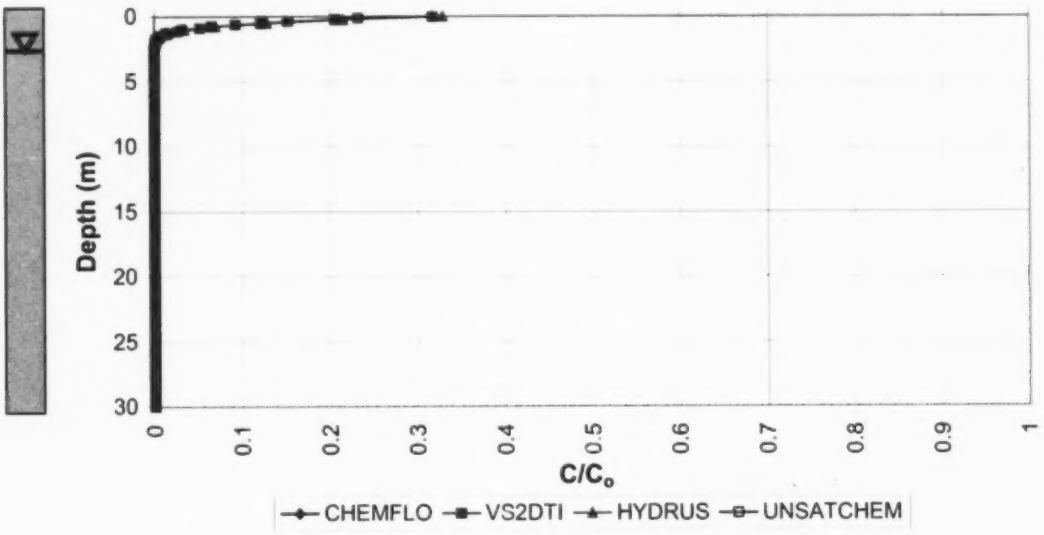


Figure B12 - Source added to a fine-grained soil column for 20 years.

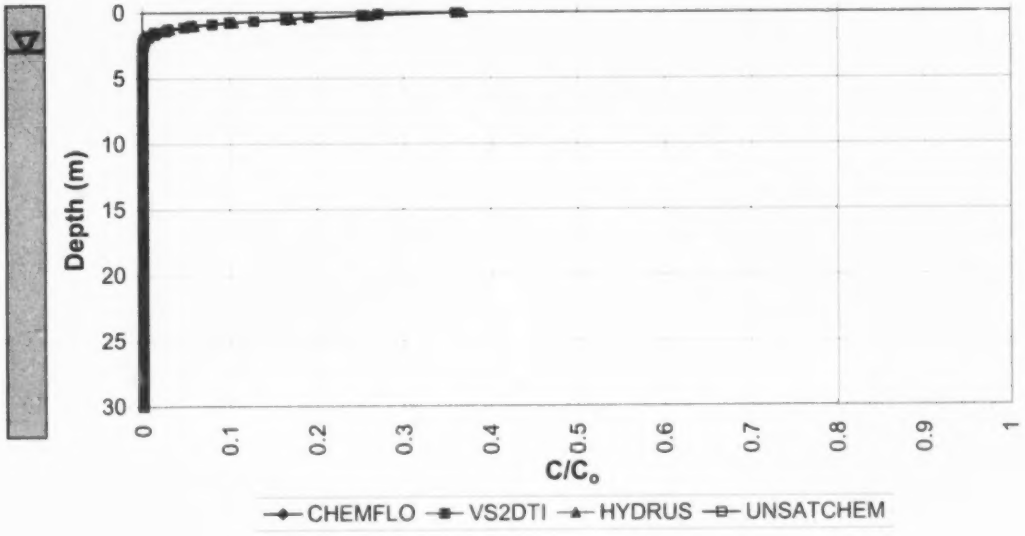


Figure B13 - Source removed from a fine-grained soil column for 5 years.

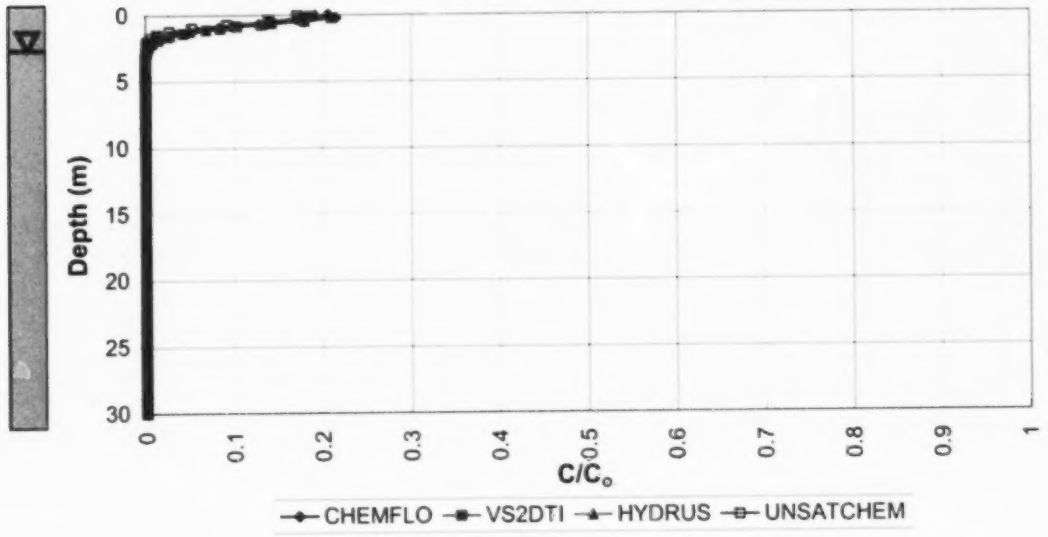


Figure B14 - Source removed from a fine-grained soil column for 10 years.

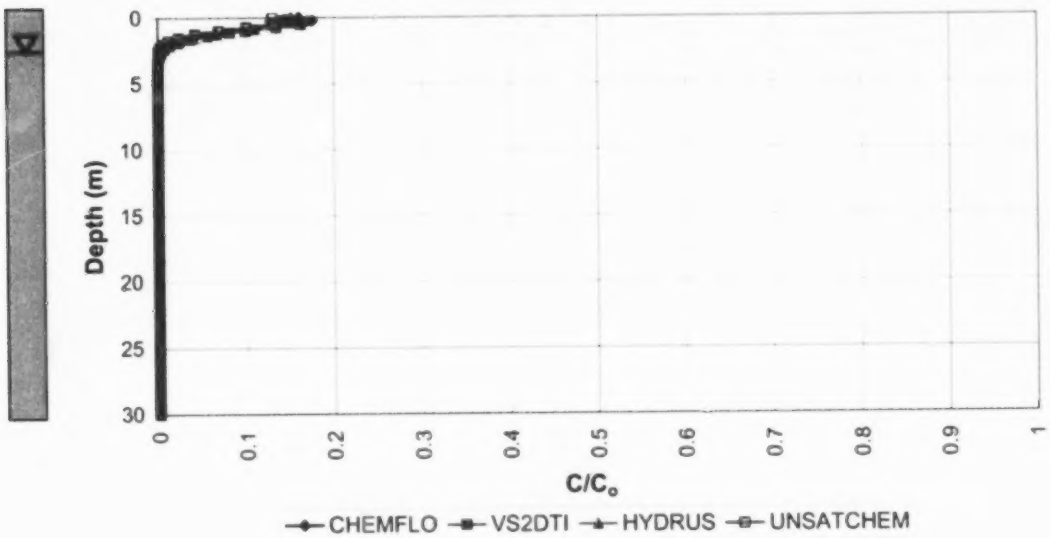


Figure B15 - Source removed from a fine-grained soil column for 15 years.

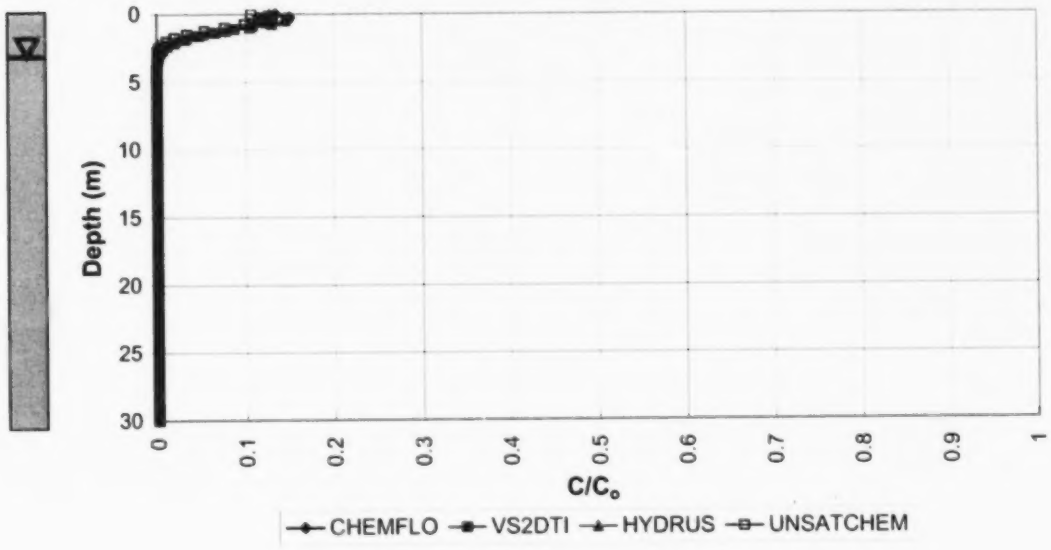


Figure B16 - Source removed from a fine-grained soil column for 20 years.

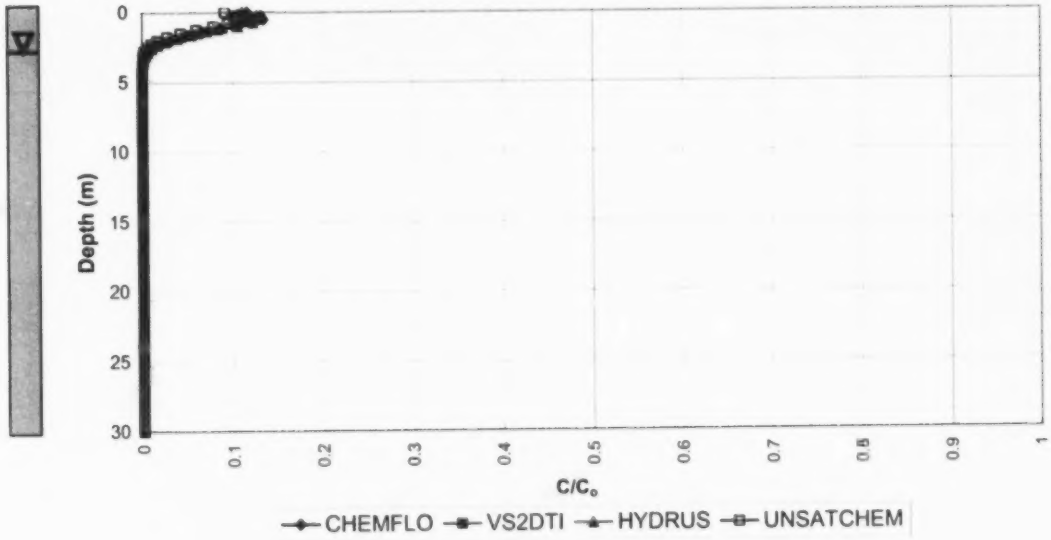


Figure B17 - Source added to a fine-coarse-fine layered column for 5 years.

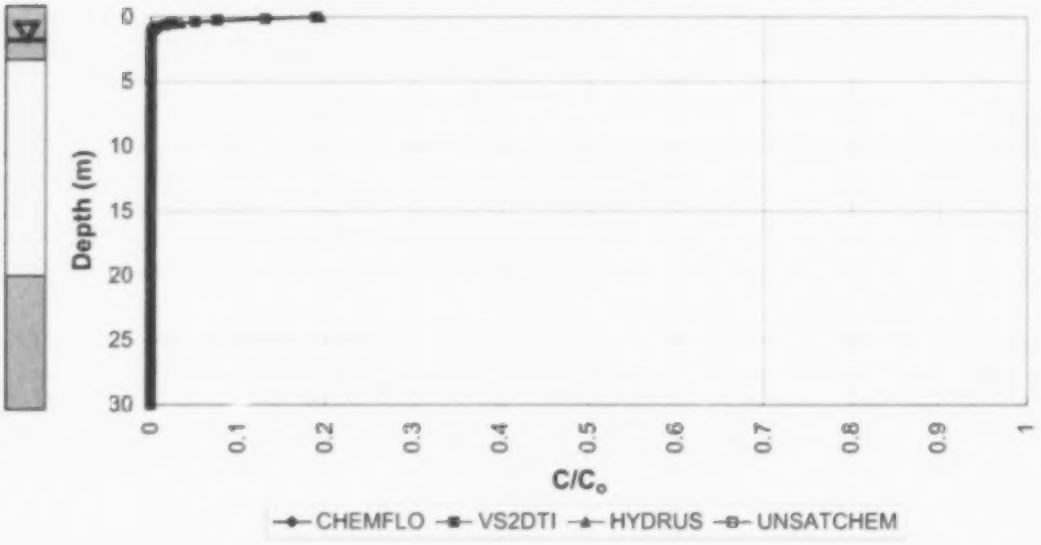


Figure B18 - Source added to a fine-coarse-fine layered column for 10 years.

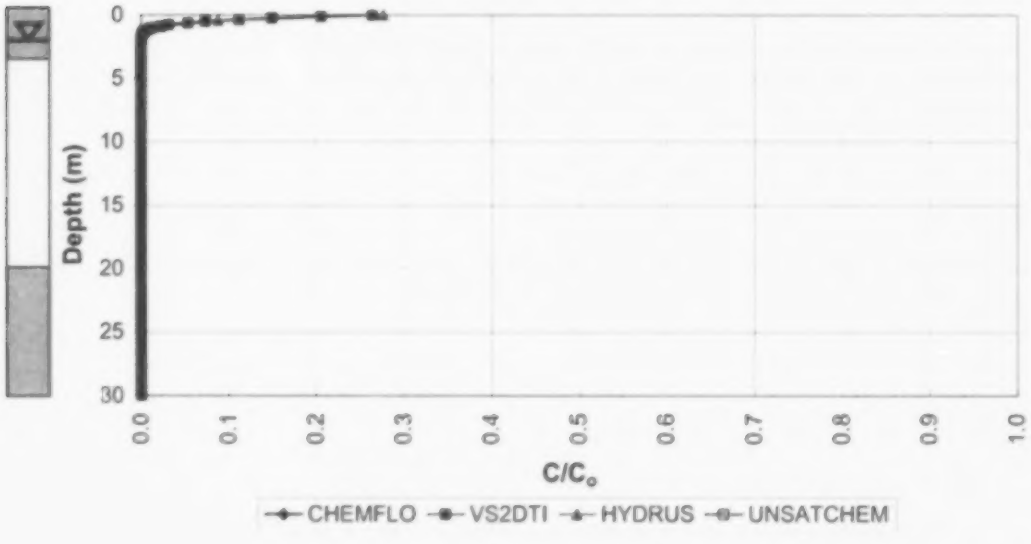


Figure B19 - Source added to a fine-coarse-fine layered column for 15 years.

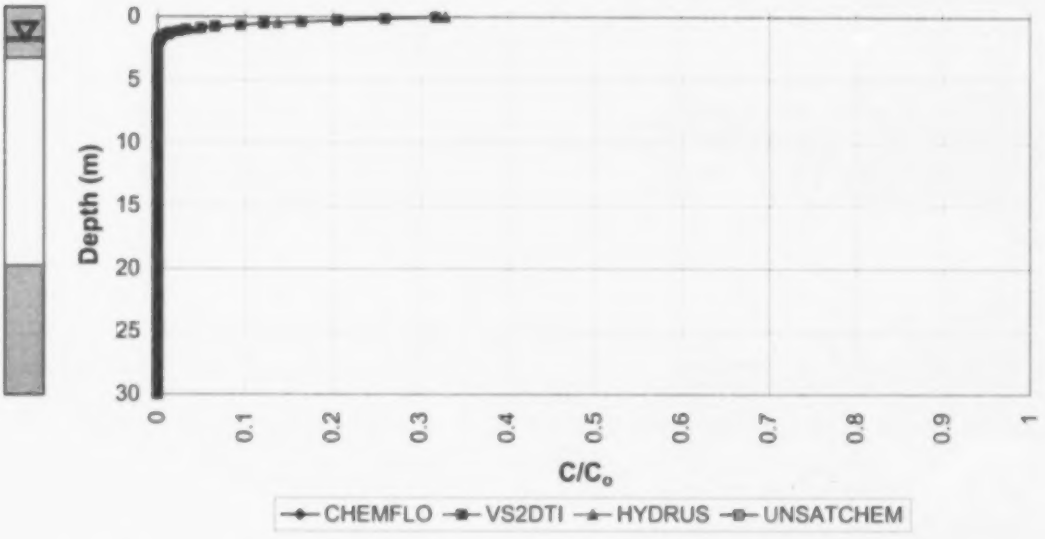


Figure B20 - Source added to a fine-coarse-fine layered column for 20 years.

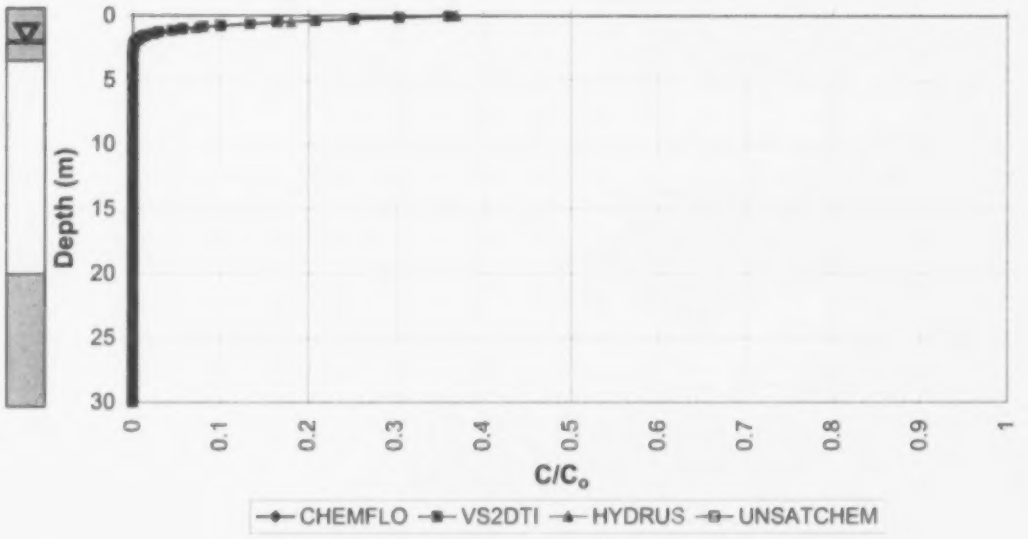


Figure B21 - Source removed from a fine-coarse-fine layered column for 5 years

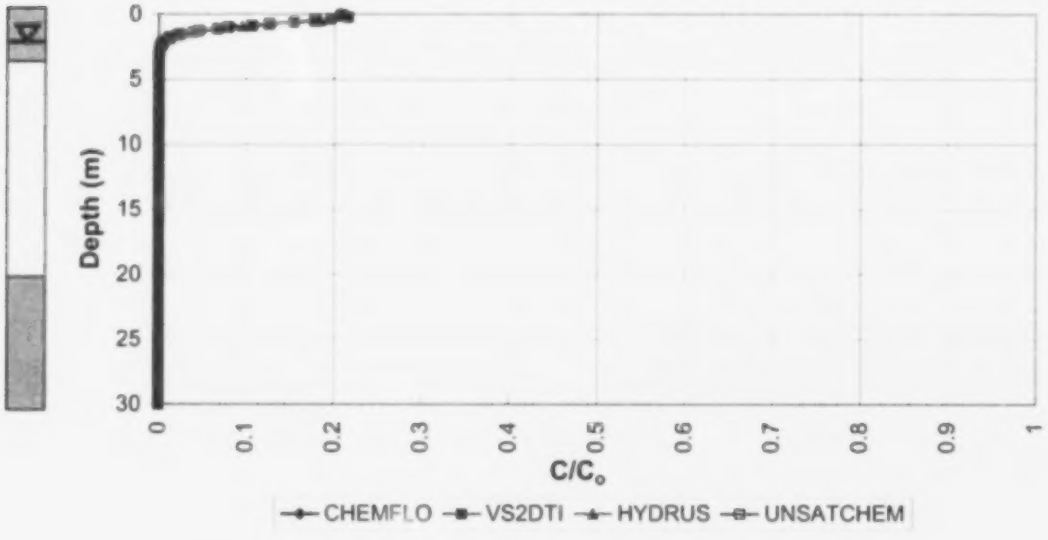


Figure B22 - Source removed from a fine-coarse-fine layered column for 10 years.

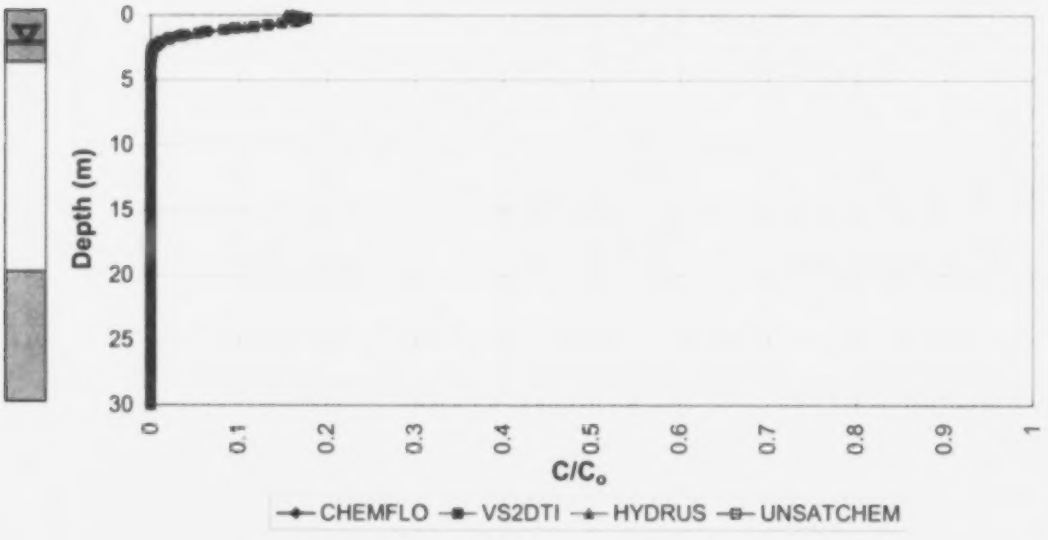


Figure B23 - Source removed from a fine-coarse-fine layered column for 15 years.

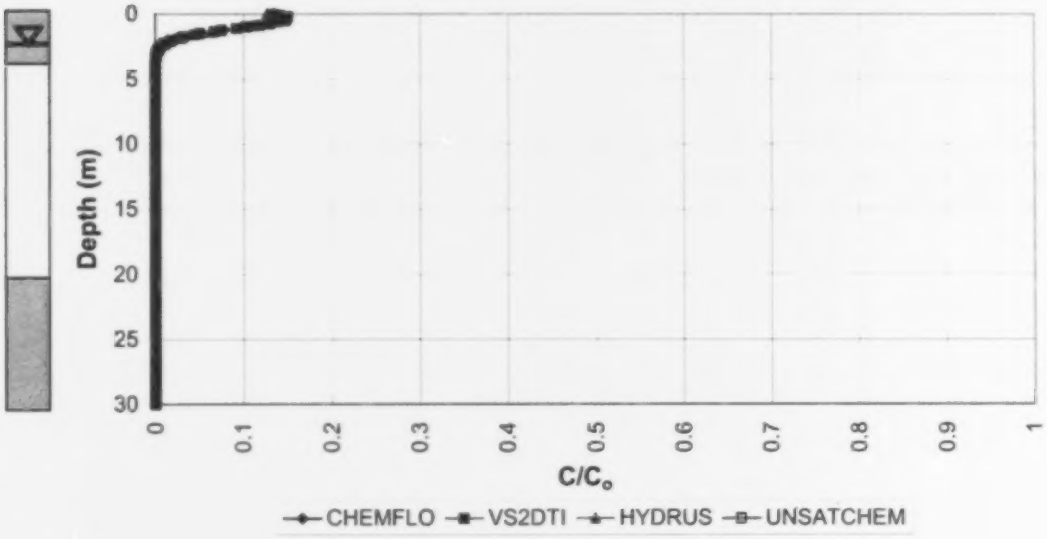


Figure B24 - Source removed from a fine-coarse-fine layered column for 20 years.

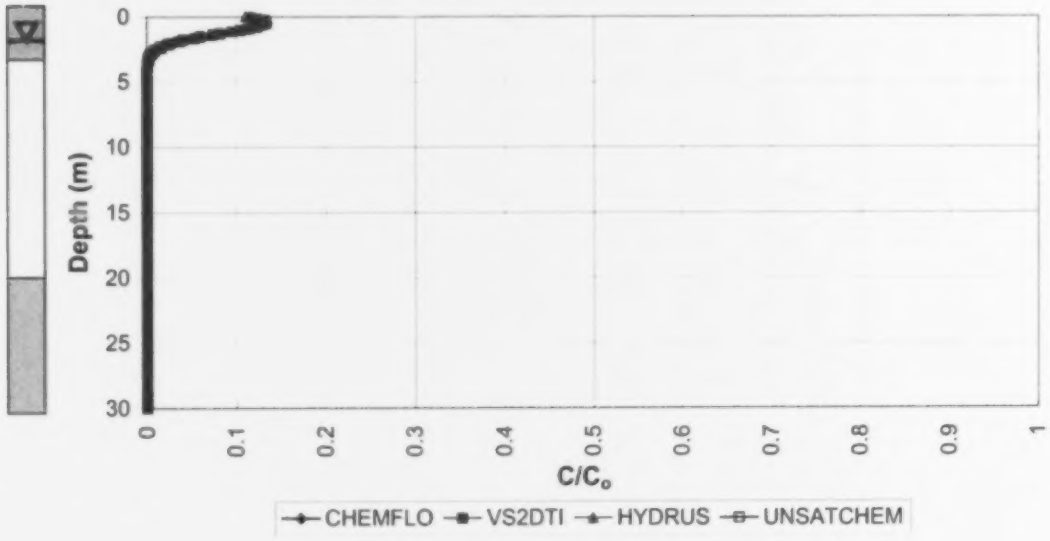


Figure B25 - Source added to a coarse-fine-coarse layered column for 5 years.

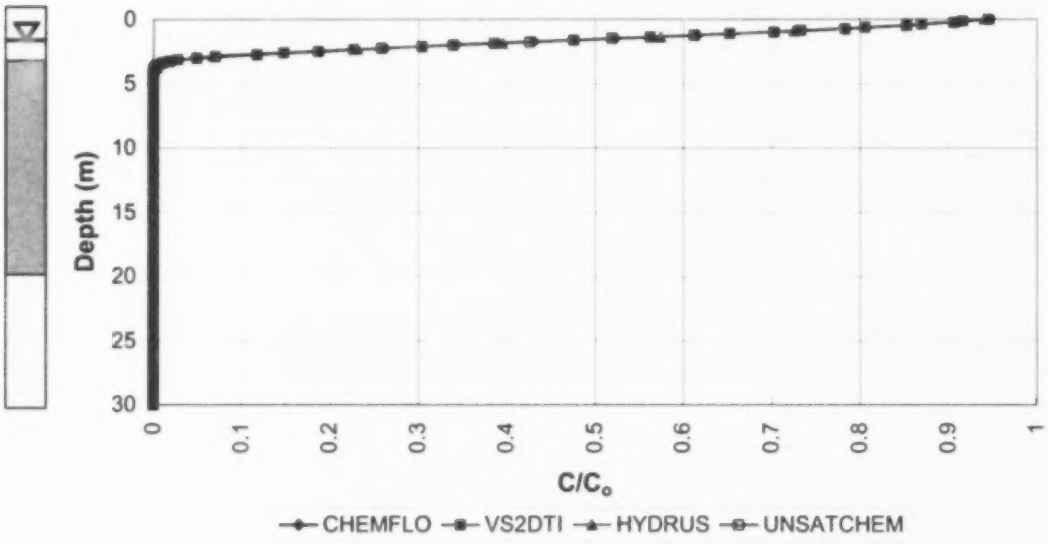


Figure B26 - Source added to a coarse-fine-coarse layered column for 10 years.

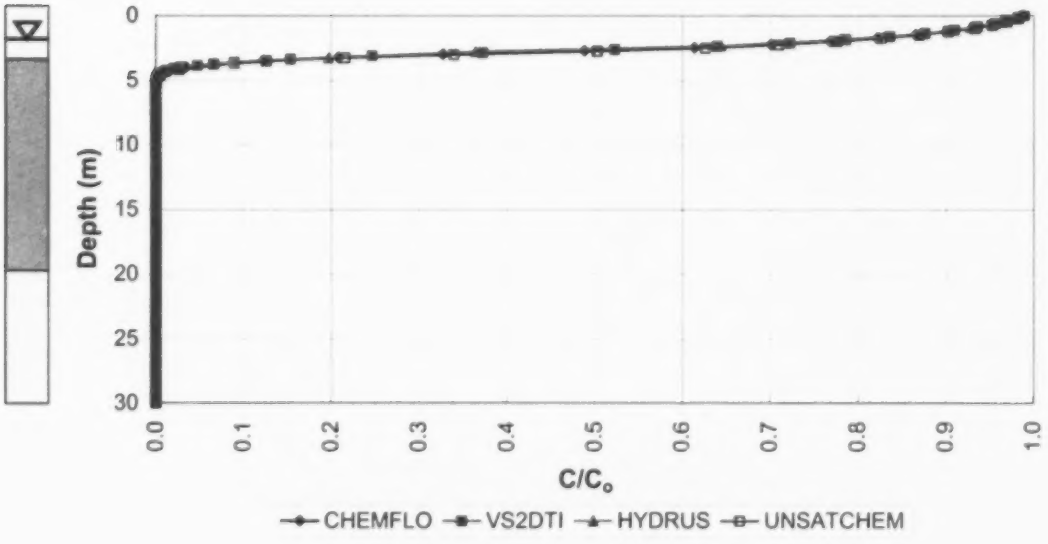


Figure B27 - Source added to a coarse-fine-coarse layered column for 15 years.

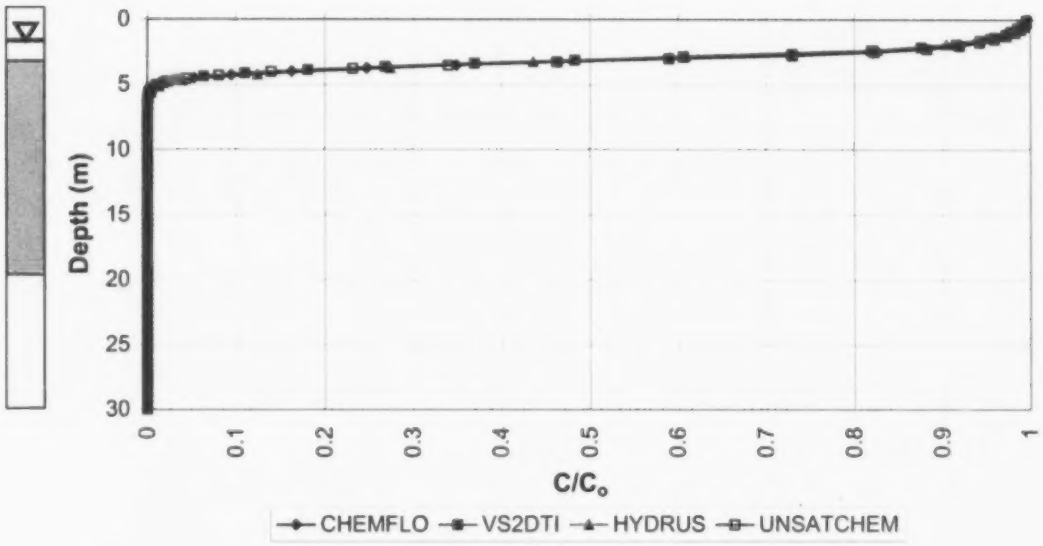


Figure B28 - Source added to a coarse-fine-coarse layered column for 20 years.

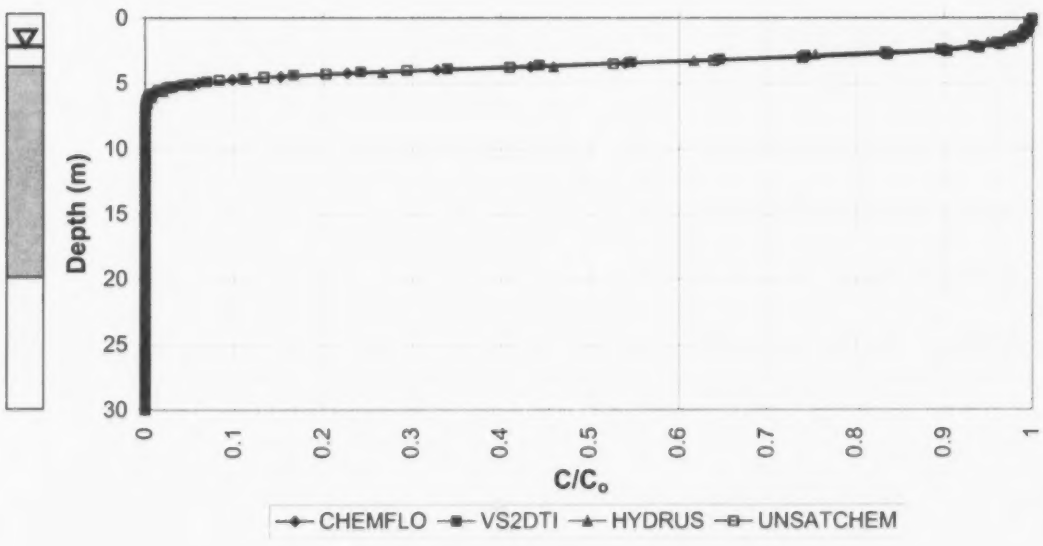


Figure B29 - Source removed from a coarse-fine-coarse layered column for 5 years.

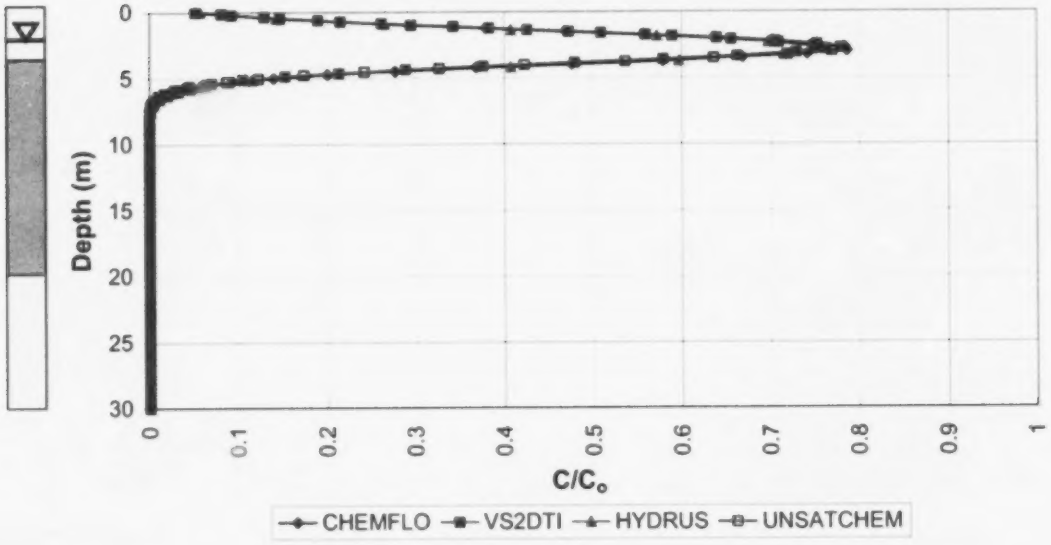


Figure B30 - Source removed from a coarse-fine-coarse layered column for 10 years.

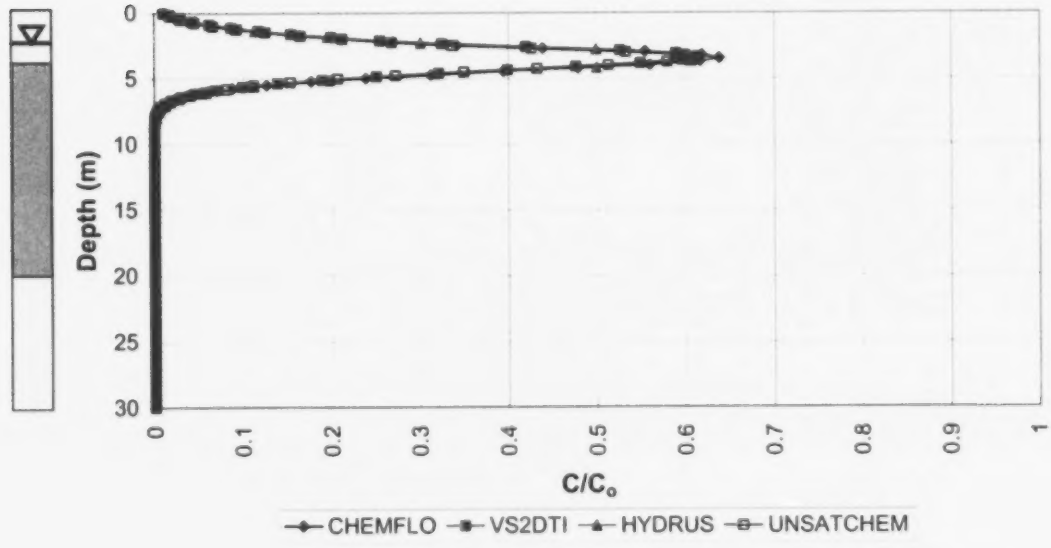


Figure B31 - Source removed from a coarse-fine-coarse layered column for 15 years.

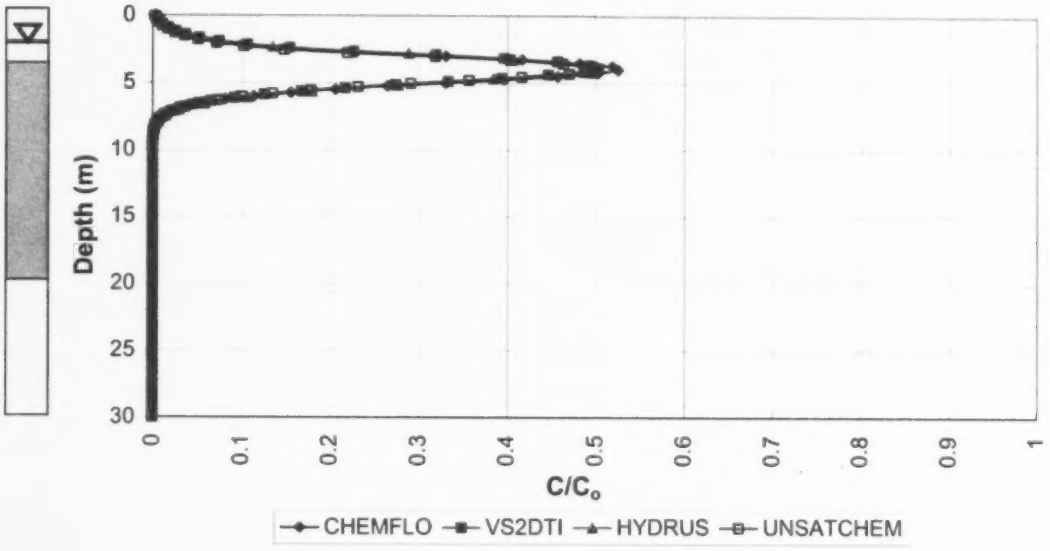


Figure B32 - Source removed from a coarse-fine-coarse layered column for 20 years.

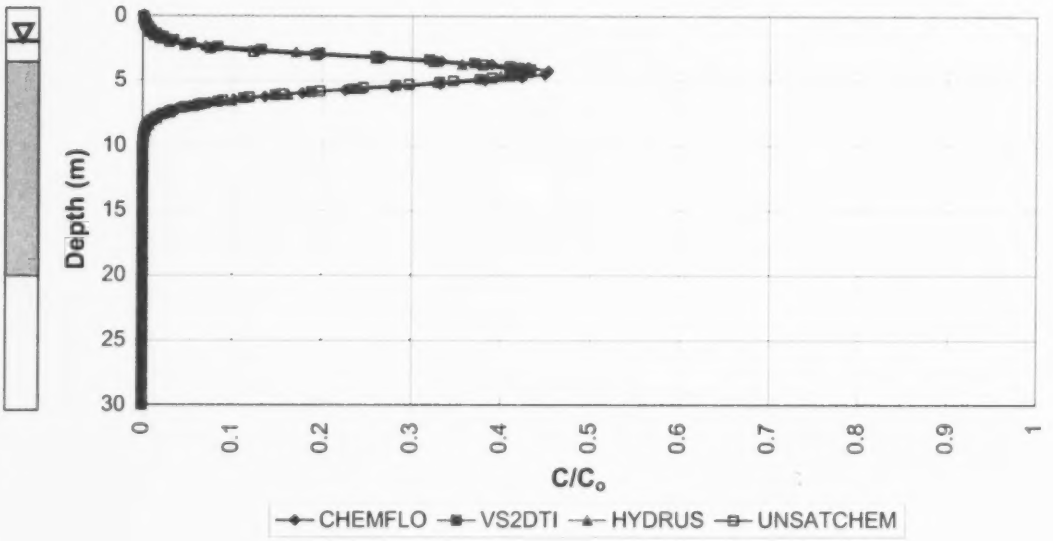


Figure B33 - Distributed source on a coarse-fine-coarse layered column year 0.

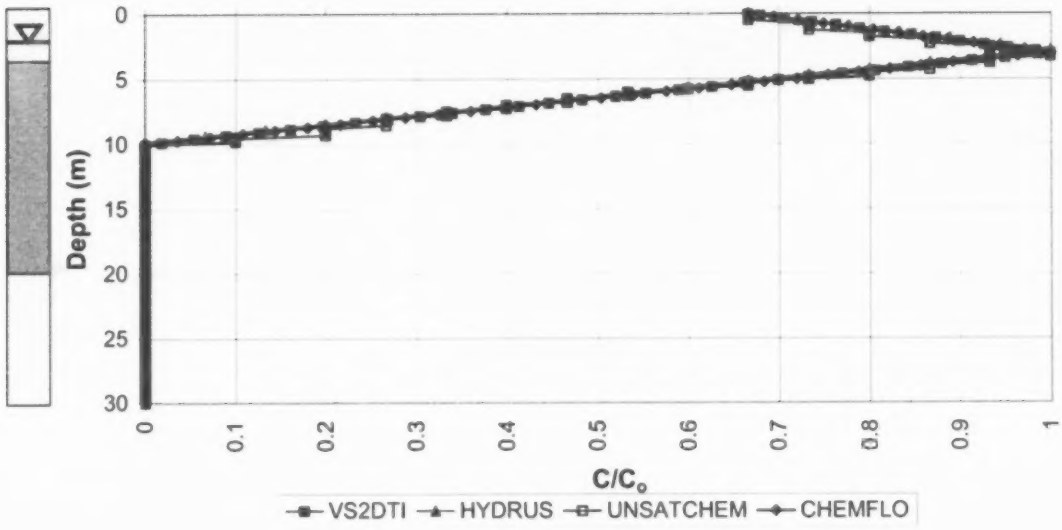


Figure B34 - Distributed source on a coarse-fine-coarse layered column year 5.

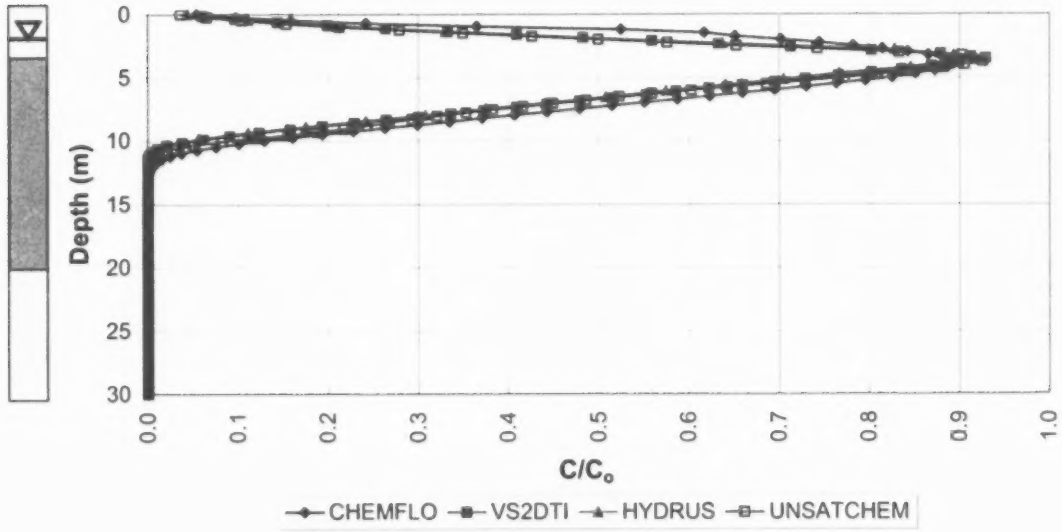


Figure B35 - Distributed source on a coarse-fine-coarse layered column year 10.

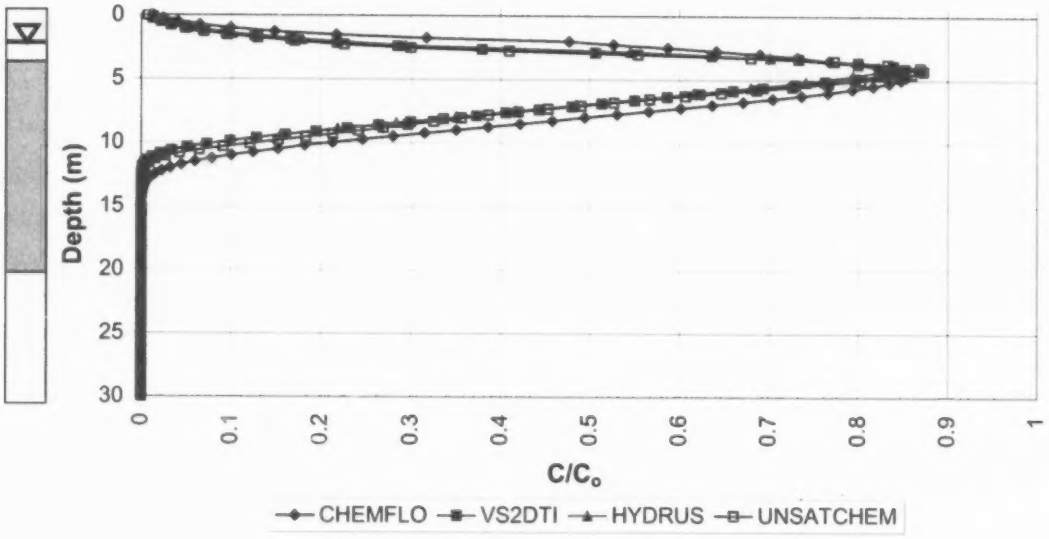
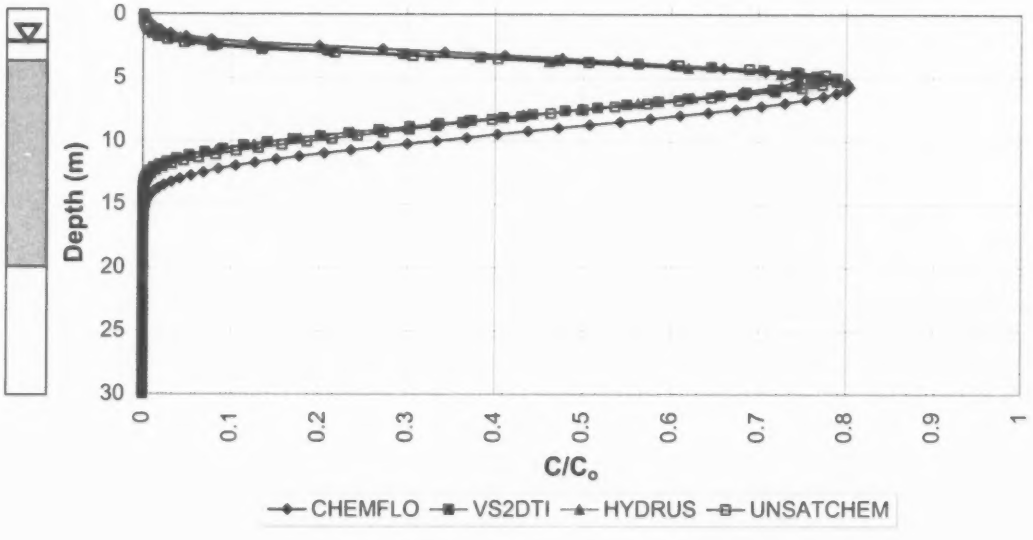


Figure B36 - Distributed source on a coarse-fine-coarse layered column year 20.



APPENDIX C

2D DETAILED OUTPUT DATA

This information was prepared by MDH Engineered Solutions Corp. (MDH) to provide a qualitative comparison of the programs HYDRUS and VS2DTI. Each program outputs the concentration data in a different format. In each program, red indicates a C/C_o of one and blue indicates a C/C_o of zero. However, the variation in contour colours between $C/C_o = 1$ and $C/C_o = 0$ are not the same. The information provided in this appendix can be used to compare the extent of the plume and the position of the peak concentration at different times.

The output for the pipeline scenario show that both codes produced comparable results. The extent of the plume and the location of the maximum concentration appear to broadly the same for both programs.

The output from the salt pile scenario also show that both codes produced comparable results. The extent of the plume and the location of the peak concentration appear to broadly similar after 20 years of source application.

Figure C1 - 2D plume for pipe line after 1 year of source application using HYDRUS.

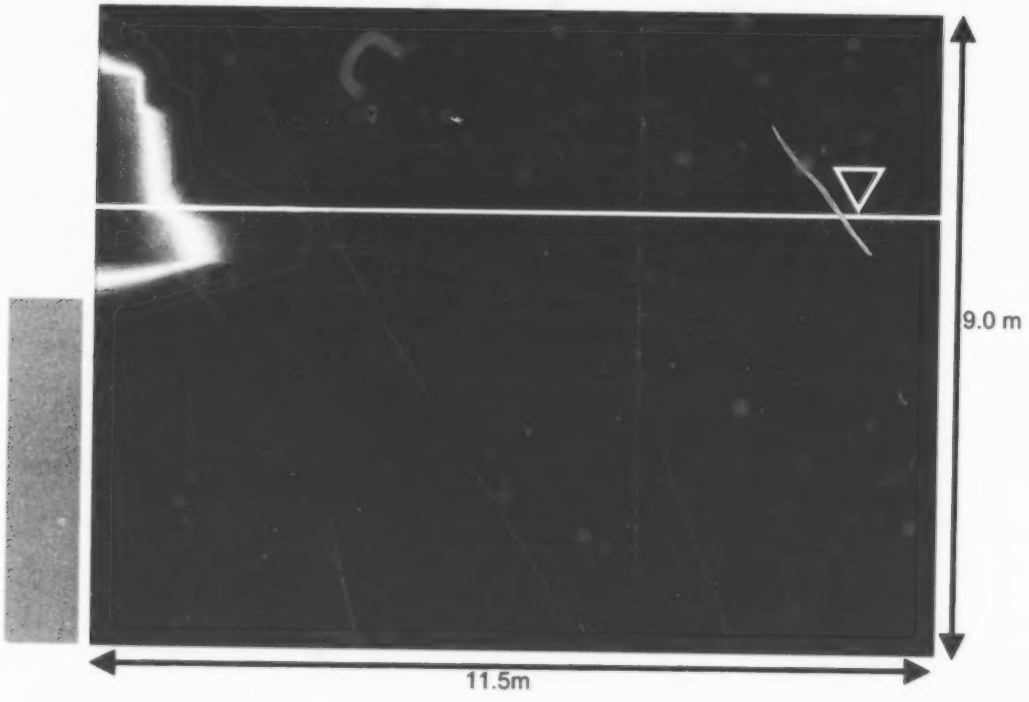


Figure C2 - 2D plume for pipe line after 1 year of source application using VS2DTI.

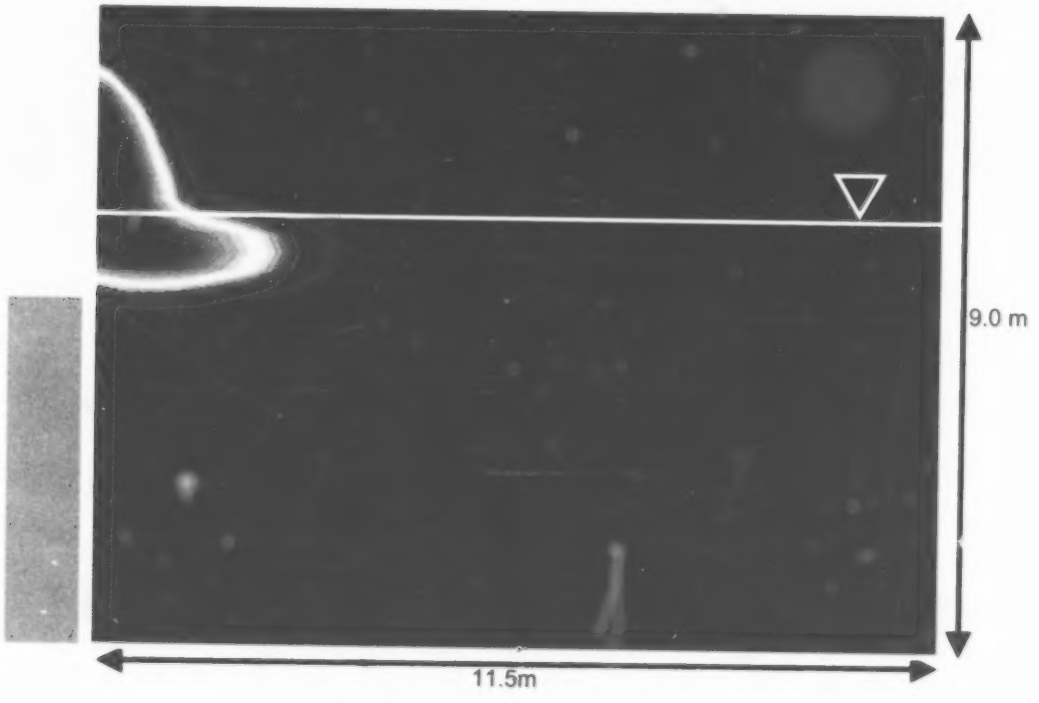


Figure C3 - 2D plume for pipe line after source removed for 5 years using HYDRUS.

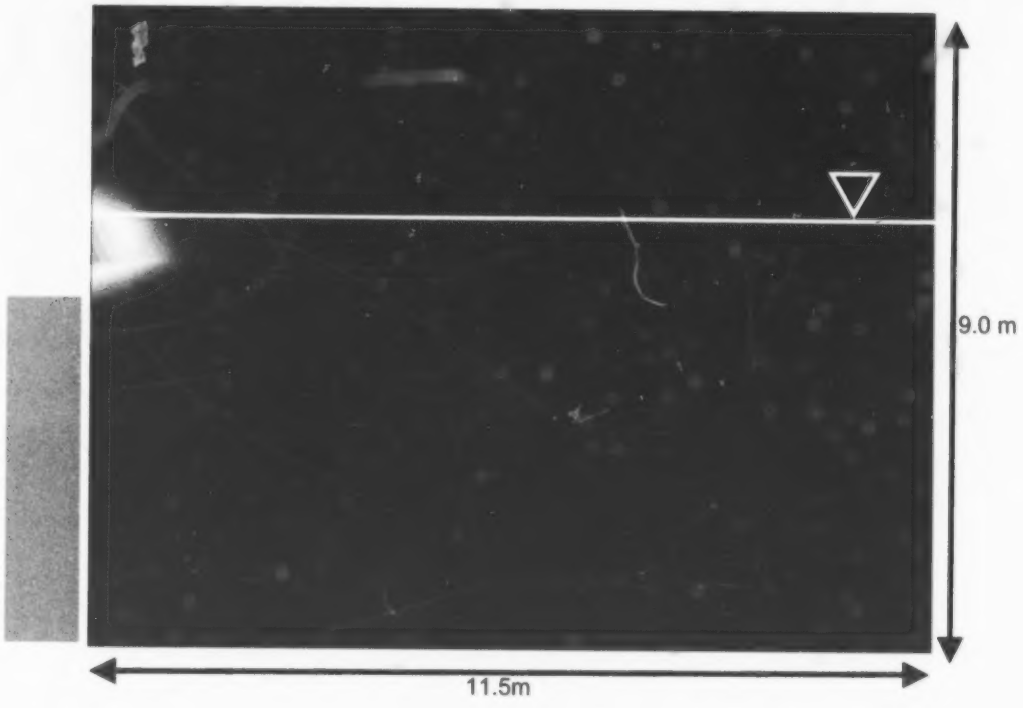


Figure C4 - 2D plume for pipe line after source removed for 5 years using VS2DIT.

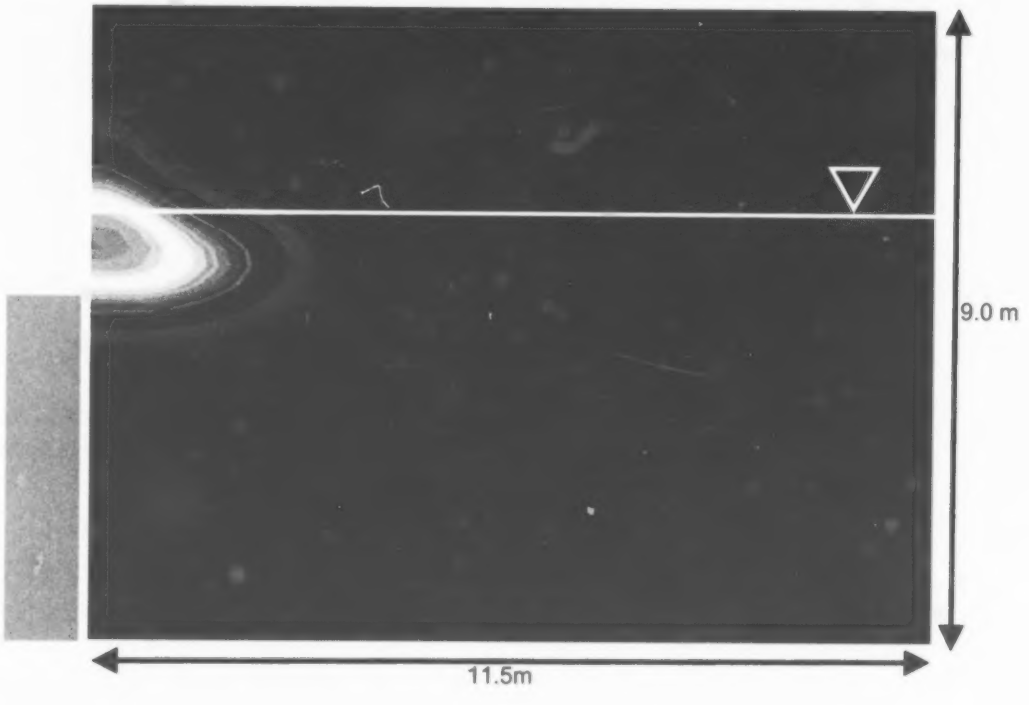


Figure C5 - 2D plume for pipe line after source removed for 10 years using HYDRUS.

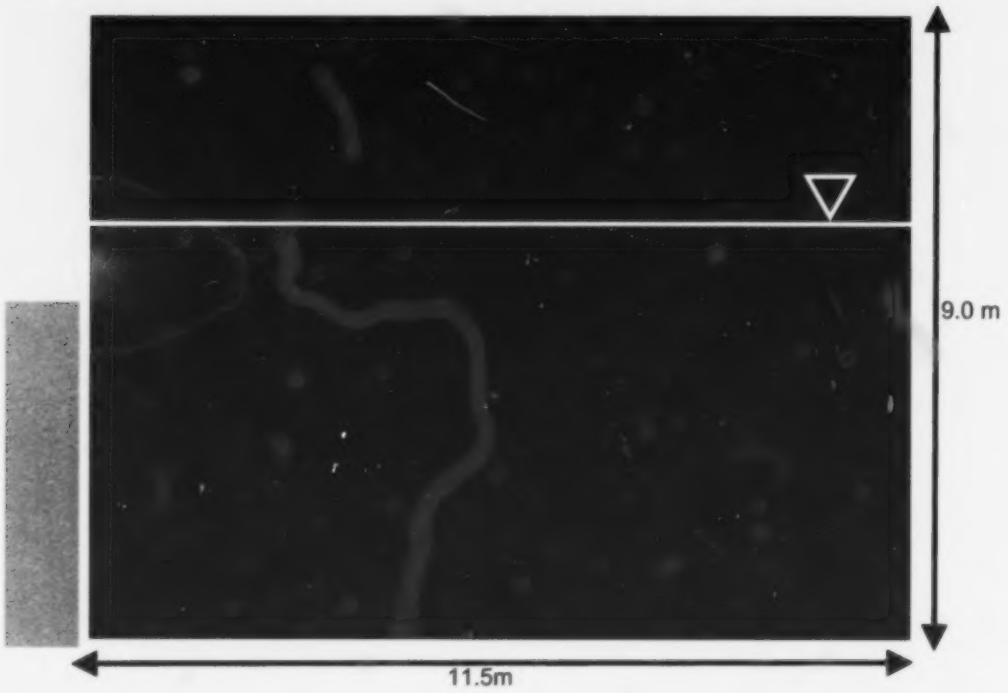


Figure C6 - 2D plume for pipe line after source removed for 10 years using VS2DTI.

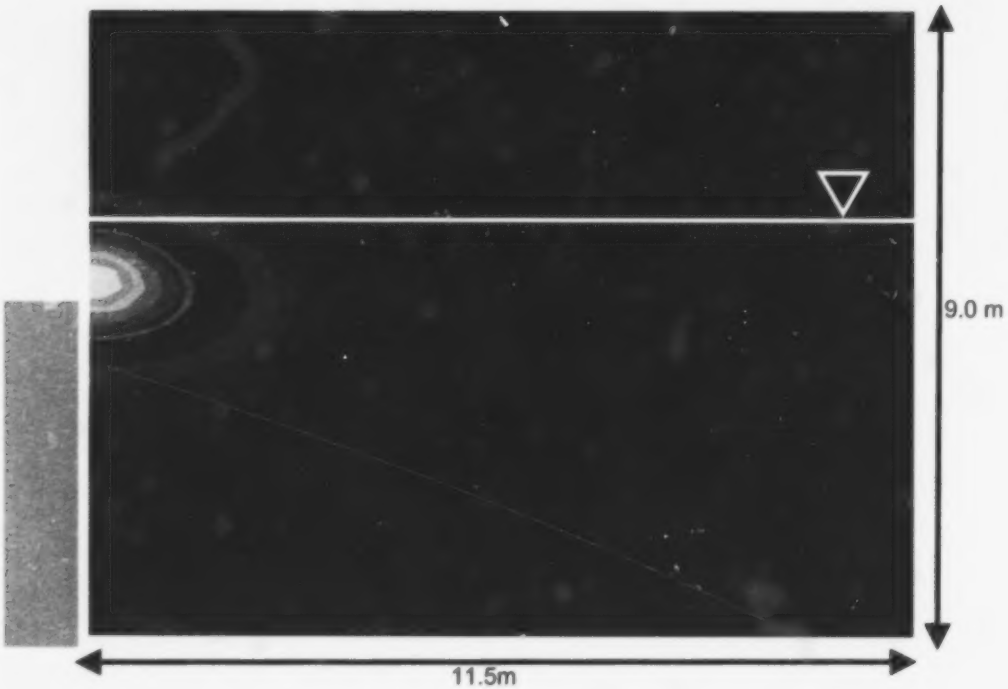


Figure C7 - 2D plume for salt pile after 20 years of source application using HYDRUS.

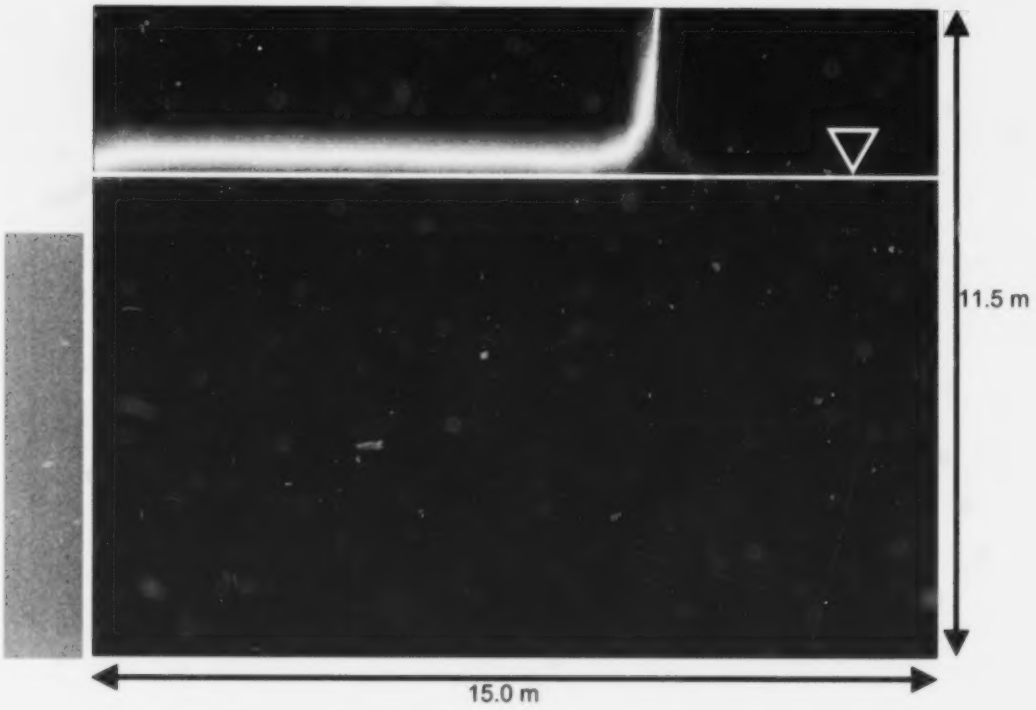


Figure C8 - 2D plume for salt pile after 20 years of source application using VS2DTI.

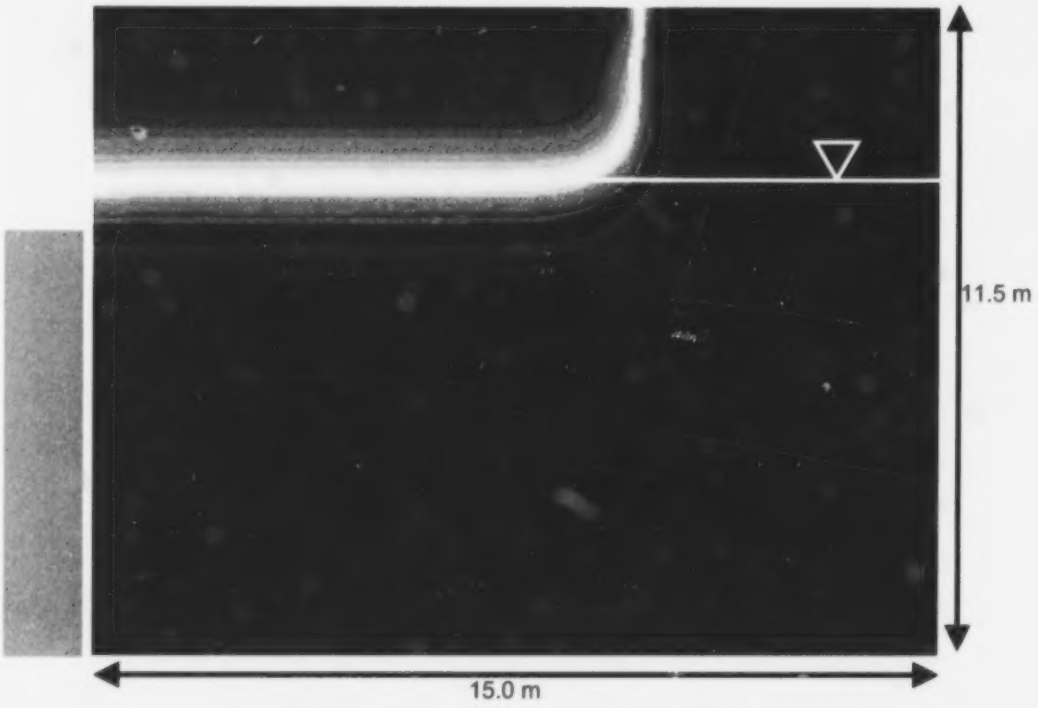


Figure C9 - 2D plume for salt pile after source removed for 10 years using HYDRUS.

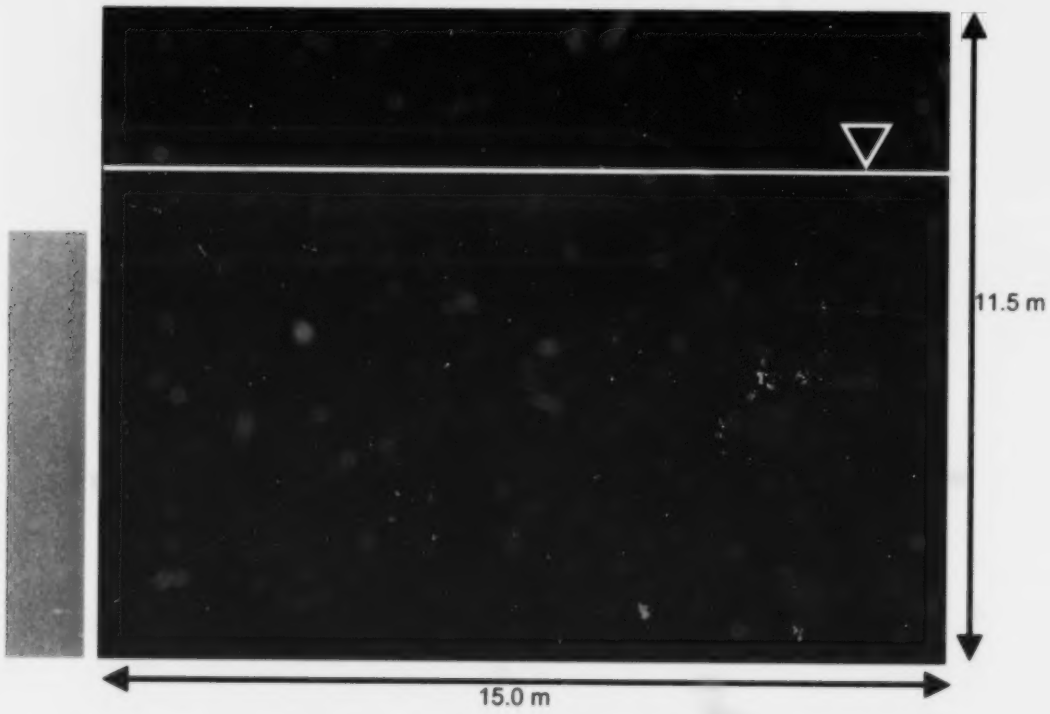


Figure C10 - 2D plume for salt pile after source removed for 10 years using VS2DIT.

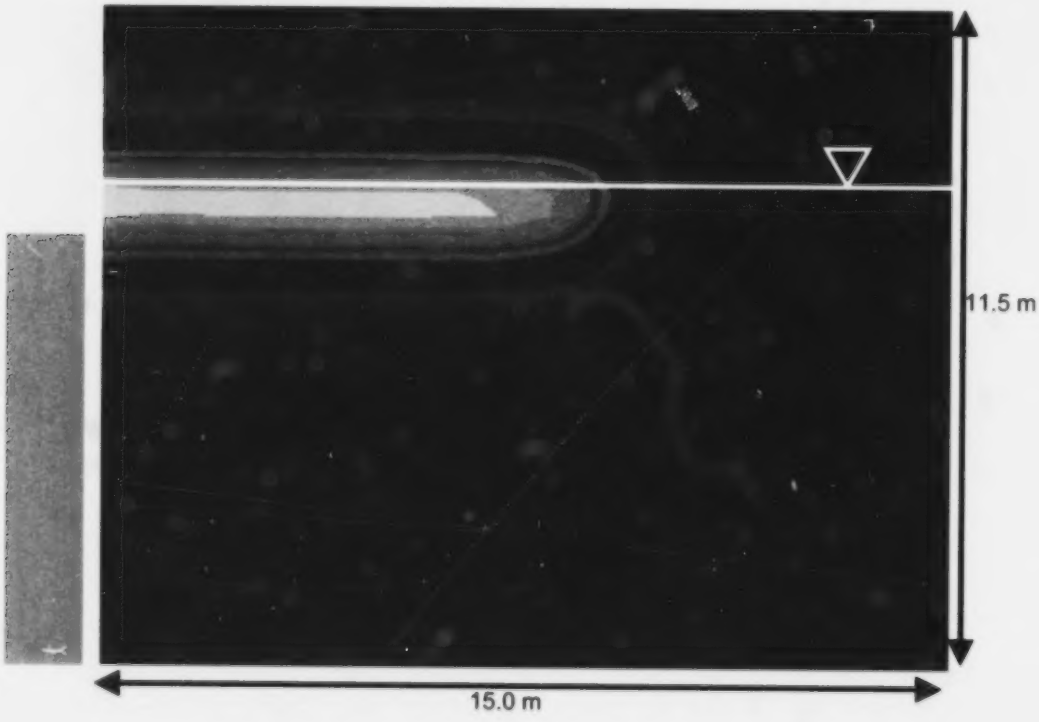


Figure C11 - 2D plume for salt pile after source removed for 20 years using HYDRUS.

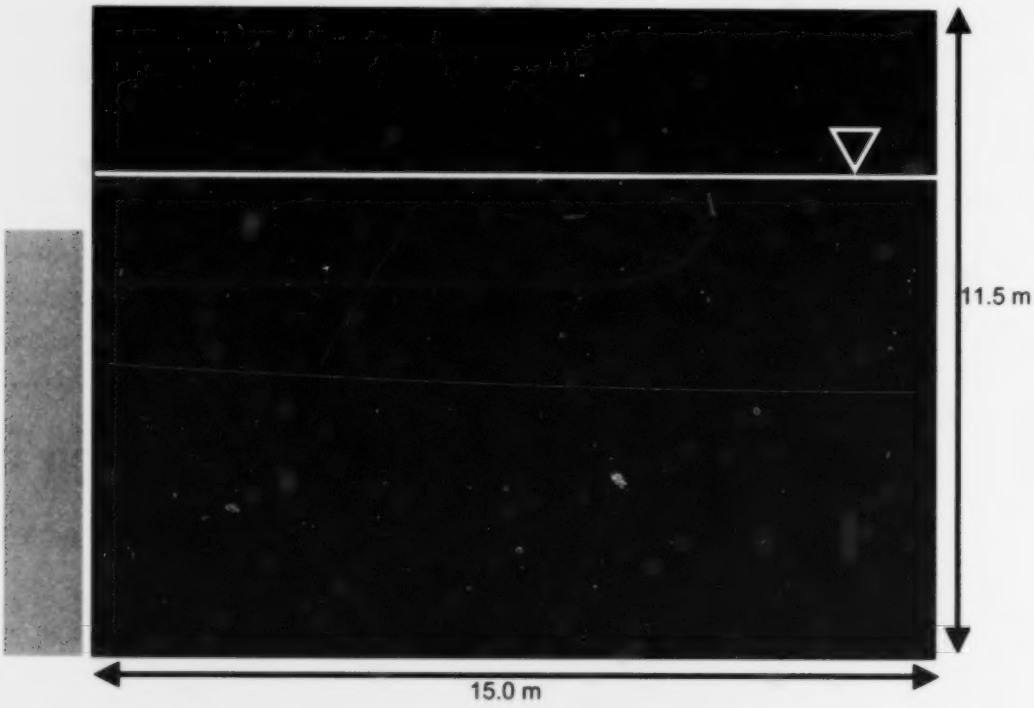
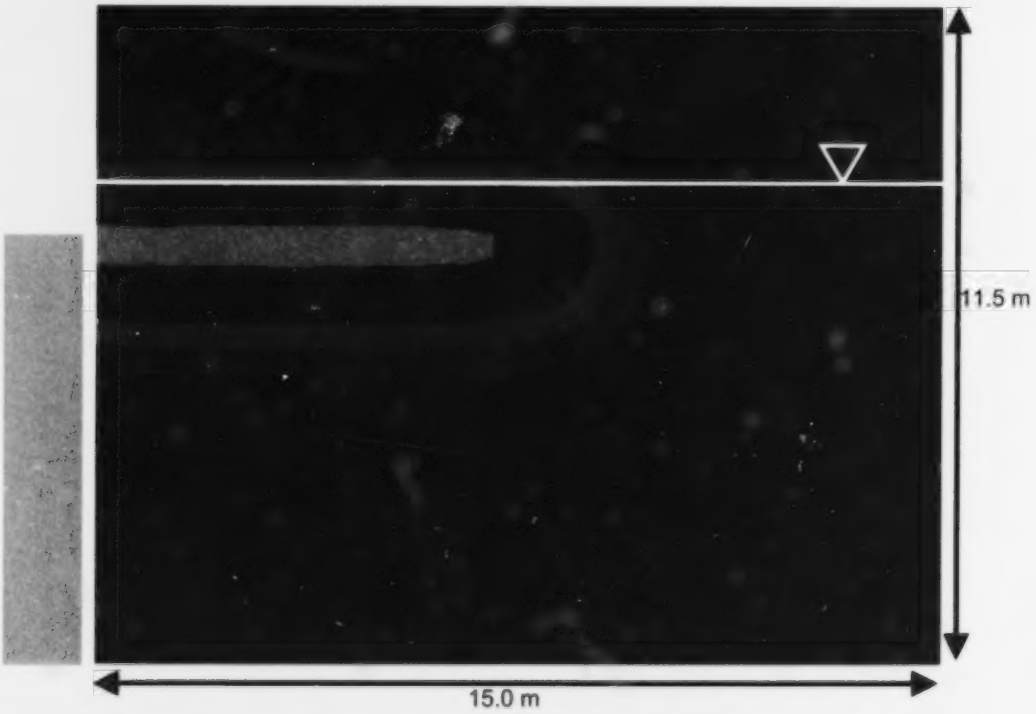


Figure C12 -2D plume for salt pile after source removed for 20 years using VS2DIT.



APPENDIX D

2D NUMERICAL ARTIFACTS

The output from the salt pile scenario completed using VS2DTI provided in this appendix show the results of a case when numerical "artifacts" were detected in a simulation. When compared with the VS2DTI results from Appendix C, the extent of the plume and the location of the peak concentration appear to broadly similar after 20 years of source application. However, the results provided in this appendix illustrate that after source cessation the simulation does not match the solution provided in Appendix C. The reason for the mismatch is that the VS2DTI results are incorrect because the grid spacing and time stepping did not satisfy necessary Peclet, Courant and Von Neumann conditions to suppress numerical "artifacts", including numerical oscillation and numerical dispersion, for the later part of the solution process. This illustrates the difficulties that might be encountered if modelling is carried out by inexperienced practitioners.

Figure D1- 2D plume for salt pile after 20 years of source application.

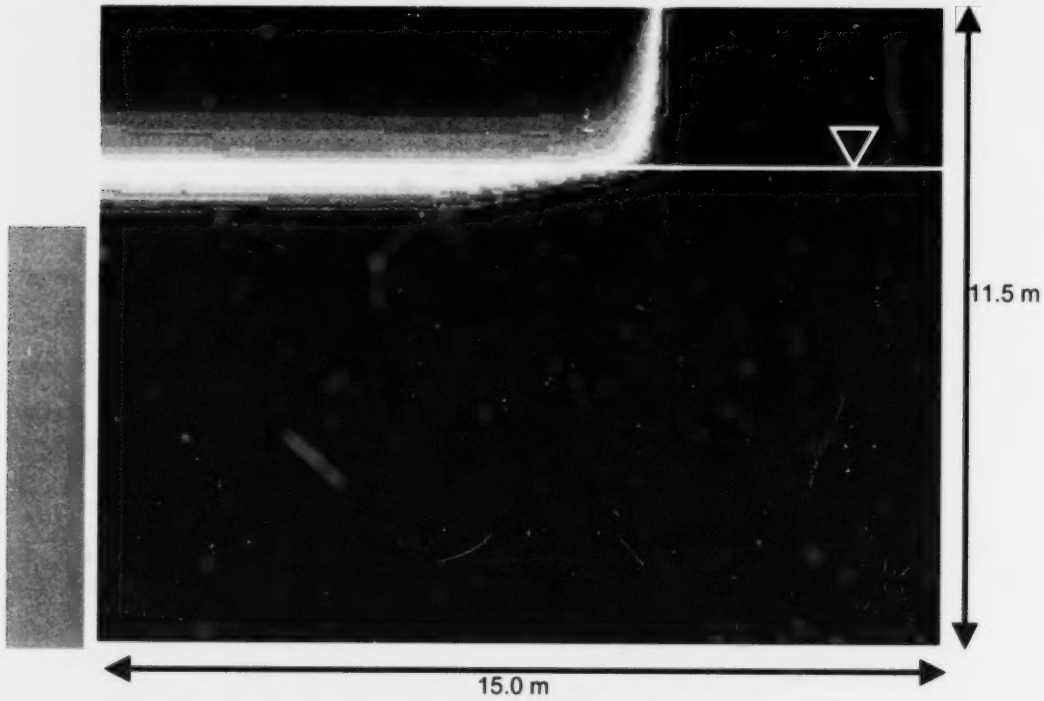


Figure D2 - 2D plume for salt pile after source removed for 10 years.

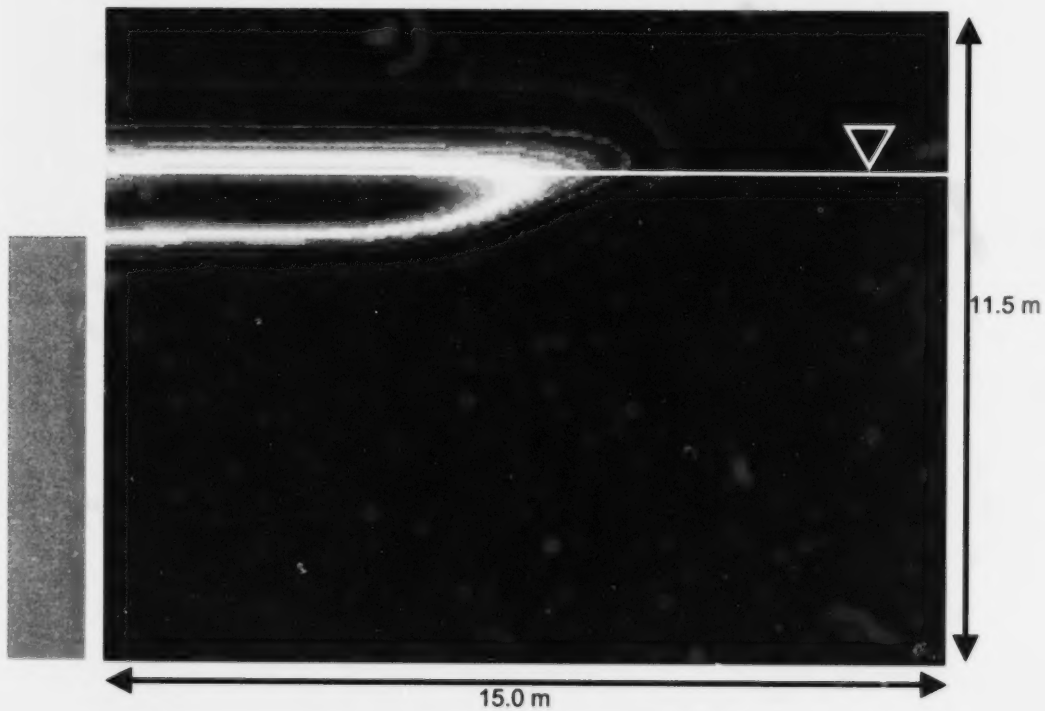


Figure D3 -2D plume for salt pile after source removed for 20 years.